



## wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 07:29 AM UTC

PDB ID : 8FWE / pdb\_00008fwe  
EMDB ID : EMD-29503  
Title : Neck structure of Agrobacterium phage Milano, C3 symmetry  
Authors : Sonani, R.R.; Wang, F.; Esteves, N.C.; Kelly, R.J.; Sebastian, A.;  
Kreutzberger, M.A.B.; Leiman, P.G.; Scharf, B.E.; Egelman, E.H.  
Deposited on : 2023-01-21  
Resolution : 3.46 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

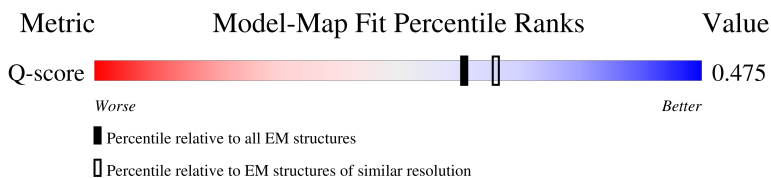
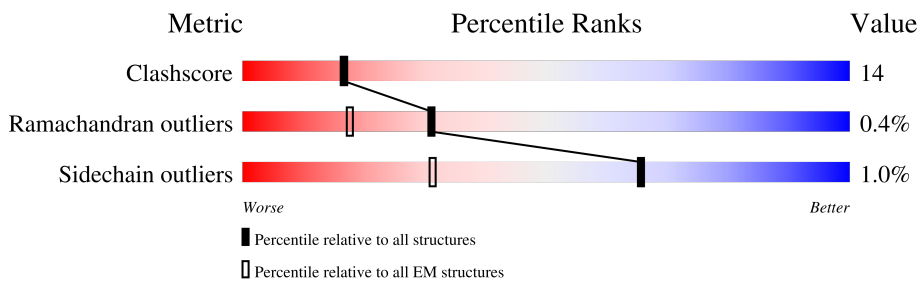
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.46 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13788 ( 2.96 - 3.96 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	230	5% (red), 73% (green), 23% (yellow), . (grey)
1	1	230	. (red), 72% (green), 24% (yellow), . (grey)
1	2	230	5% (red), 71% (green), 25% (yellow), . (grey)
1	3	230	5% (red), 72% (green), 25% (yellow), . (grey)

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Mol	Chain	Length	Quality of chain	
1	4	230	5%	72% 24% ..
1	5	230	5%	73% 23% .
1	6	230	7%	74% 23% .
1	7	230	6%	71% 25% ..
1	8	230	5%	75% 22% .
1	9	230	5%	73% 23% ..
1	A	230	6%	73% 23% .
1	B	230	5%	70% 26% .
1	C	230	5%	77% 20% .
1	D	230	6%	72% 24% .
1	E	230	5%	72% 25% .
1	F	230	7%	75% 22% .
1	G	230	5%	71% 25% ..
1	J	230	8%	72% 25% .
1	K	230	7%	77% 20% .
1	L	230	7%	75% 22% .
1	M	230	7%	74% 23% .
1	N	230	7%	75% 22% .
1	O	230	7%	69% 27% ..
1	P	230	7%	80% 17% .
1	Q	230	7%	77% 19% .
1	R	230	7%	72% 25% .
1	S	230	7%	73% 24% .
1	T	230	7%	70% 26% .
1	U	230	7%	78% 19% .

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Mol	Chain	Length	Quality of chain	
1	V	230	6%	75% 22%
1	W	230	7%	73% 23%
1	X	230	8%	73% 23%
1	Y	230	.	74% 23%
1	Z	230	.	76% 21%
1	a	230	5%	71% 26%
1	b	230	6%	68% 29%
1	c	230	5%	73% 24%
1	d	230	.	73% 24%
1	e	230	5%	74% 23%
1	f	230	5%	69% 28%
1	g	230	6%	67% 30%
1	h	230	6%	70% 27%
1	i	230	.	73% 24%
1	j	230	6%	72% 24%
1	k	230	5%	72% 25%
1	l	230	6%	67% 30%
1	m	230	5%	74% 23%
1	n	230	.	72% 24%
1	o	230	.	75% 22%
1	p	230	.	74% 22%
1	q	230	.	72% 24%
1	r	230	5%	72% 24%
1	s	230	5%	73% 24%
1	t	230	.	76% 21%

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Mol	Chain	Length	Quality of chain
1	u	230	72% 24%
1	v	230	73% 24%
1	w	230	72% 24%
1	x	230	5% 75% 21%
1	y	230	75% 22%
1	z	230	73% 23%
2	AA	420	27% 61% 30% 9%
2	AB	420	33% 57% 34% 9%
2	AC	420	32% 57% 33% 9%
2	AD	420	25% 56% 33% 9%
2	AE	420	26% 59% 31% 9%
2	AF	420	33% 57% 32% 9%
2	AG	420	31% 59% 31% 9%
2	AH	420	25% 56% 33% 9%
2	AI	420	26% 58% 32% 9%
2	AJ	420	34% 56% 34% 9%
2	AK	420	32% 62% 29% 9%
2	AL	420	25% 55% 35% 9%
3	AM	141	62% 27% 11%
3	AN	141	61% 26% 11%
3	AO	141	62% 26% 11%
3	AP	141	55% 32% 11%
3	H	141	59% 28% 11%
3	I	141	59% 28% 11%
4	AQ	178	67% 18% 13%

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Mol	Chain	Length	Quality of chain
4	AR	178	65% 19% 13%
4	AS	178	66% 19% 13%
4	AT	178	65% 21% 13%
4	AW	178	67% 19% 13%
4	AX	178	66% 20% 13%
5	AU	136	63% 30% 6%
5	AV	136	62% 32% 6%
5	AY	136	62% 32% 6%
5	AZ	136	67% 26% 6%
5	Aa	136	63% 30% 6%
5	Ab	136	69% 24% 6%
6	R3	202	55% 31% 10% 8%
6	R4	202	54% 30% 10% 6%
6	R5	202	50% 36% 10% 8%
6	S3	202	51% 36% 11% 5%
6	S4	202	51% 35% 11% 5%
6	S5	202	53% 33% 11% 7%
6	T3	202	58% 30% 11% 12%
6	T4	202	53% 32% 11% 12%
6	T5	202	56% 31% 11% 12%
6	U3	202	57% 27% 11% 12%
6	U4	202	48% 35% 11% 10%
6	U5	202	56% 30% 11% 11%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 171990 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Collar sheath protein, gp13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	J	223	1679	1065	279	327	8	0	0
1	K	223	1679	1065	279	327	8	0	0
1	L	223	1679	1065	279	327	8	0	0
1	M	223	1679	1065	279	327	8	0	0
1	N	223	1679	1065	279	327	8	0	0
1	O	223	1679	1065	279	327	8	0	0
1	P	223	1679	1065	279	327	8	0	0
1	Q	223	1679	1065	279	327	8	0	0
1	R	223	1679	1065	279	327	8	0	0
1	S	223	1679	1065	279	327	8	0	0
1	T	223	1679	1065	279	327	8	0	0
1	U	223	1679	1065	279	327	8	0	0
1	V	223	1679	1065	279	327	8	0	0
1	W	223	1679	1065	279	327	8	0	0
1	X	223	1679	1065	279	327	8	0	0
1	Y	223	1679	1065	279	327	8	0	0
1	Z	223	1679	1065	279	327	8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	b	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	c	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	d	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	e	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	f	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	g	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	h	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	i	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	j	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	k	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	l	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	m	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	n	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	o	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	p	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	q	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	r	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	s	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	t	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	u	223	Total 1679	C 1065	N 279	O 327	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	v	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	w	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	x	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	y	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	z	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	1	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	2	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	4	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	5	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	6	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	7	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	8	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	9	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	0	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	A	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	B	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	C	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	D	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	E	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
1	F	223	Total 1679	C 1065	N 279	O 327	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		

- Molecule 2 is a protein called Portal protein, gp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AA	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AB	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AC	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AD	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AE	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AF	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AG	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AH	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AI	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AJ	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AK	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AL	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		

- Molecule 3 is a protein called Neck 2 protein, gp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AM	125	Total	C	N	O	S	0	0
			997	621	183	185	8		
3	AP	125	Total	C	N	O	S	0	0
			997	621	183	185	8		
3	AN	125	Total	C	N	O	S	0	0
			997	621	183	185	8		
3	H	125	Total	C	N	O	S	0	0
			997	621	183	185	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	AO	125	Total	C	N	O	S	0	0
			997	621	183	185	8		
3	I	125	Total	C	N	O	S	0	0
			997	621	183	185	8		

- Molecule 4 is a protein called Tail-terminator protein, gp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AQ	155	Total	C	N	O	S	0	0
			1251	798	207	243	3		
4	AR	155	Total	C	N	O	S	0	0
			1251	798	207	243	3		
4	AS	155	Total	C	N	O	S	0	0
			1251	798	207	243	3		
4	AT	155	Total	C	N	O	S	0	0
			1251	798	207	243	3		
4	AW	155	Total	C	N	O	S	0	0
			1251	798	207	243	3		
4	AX	155	Total	C	N	O	S	0	0
			1251	798	207	243	3		

- Molecule 5 is a protein called Tail-tube, gp21.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AU	128	Total	C	N	O	S	0	0
			977	606	162	202	7		
5	AZ	128	Total	C	N	O	S	0	0
			977	606	162	202	7		
5	AV	128	Total	C	N	O	S	0	0
			977	606	162	202	7		
5	Aa	128	Total	C	N	O	S	0	0
			977	606	162	202	7		
5	AY	128	Total	C	N	O	S	0	0
			977	606	162	202	7		
5	Ab	128	Total	C	N	O	S	0	0
			977	606	162	202	7		

- Molecule 6 is a protein called Neck 1 protein, gp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R3	181	Total	C	N	O	S	0	0
			1395	887	249	255	4		

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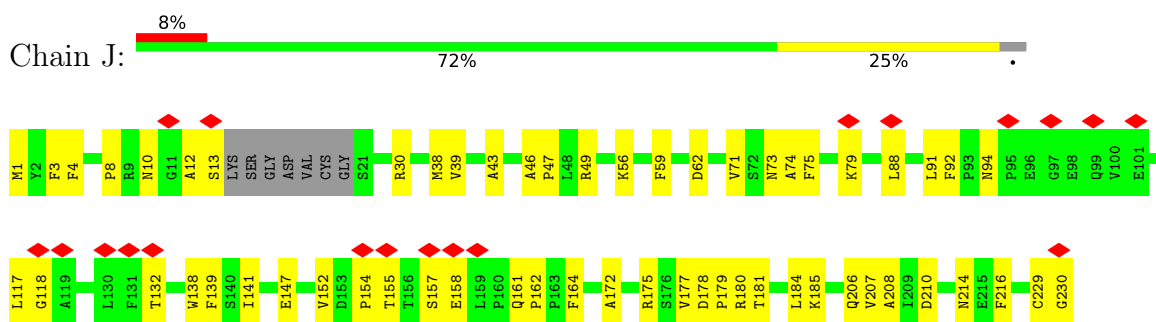
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Mol	Chain	Residues	Atoms					AltConf	Trace
6	S3	180	Total	C	N	O	S	0	0
			1387	881	248	254	4		
6	T3	179	Total	C	N	O	S	0	0
			1379	875	247	253	4		
6	U3	180	Total	C	N	O	S	0	0
			1387	881	248	254	4		
6	R4	181	Total	C	N	O	S	0	0
			1395	887	249	255	4		
6	S4	180	Total	C	N	O	S	0	0
			1387	881	248	254	4		
6	T4	179	Total	C	N	O	S	0	0
			1379	875	247	253	4		
6	U4	180	Total	C	N	O	S	0	0
			1387	881	248	254	4		
6	R5	181	Total	C	N	O	S	0	0
			1395	887	249	255	4		
6	S5	180	Total	C	N	O	S	0	0
			1387	881	248	254	4		
6	T5	179	Total	C	N	O	S	0	0
			1379	875	247	253	4		
6	U5	180	Total	C	N	O	S	0	0
			1387	881	248	254	4		

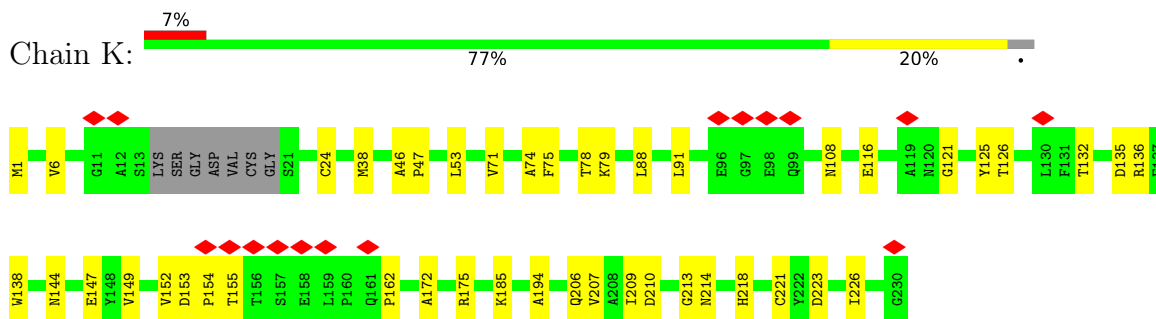
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

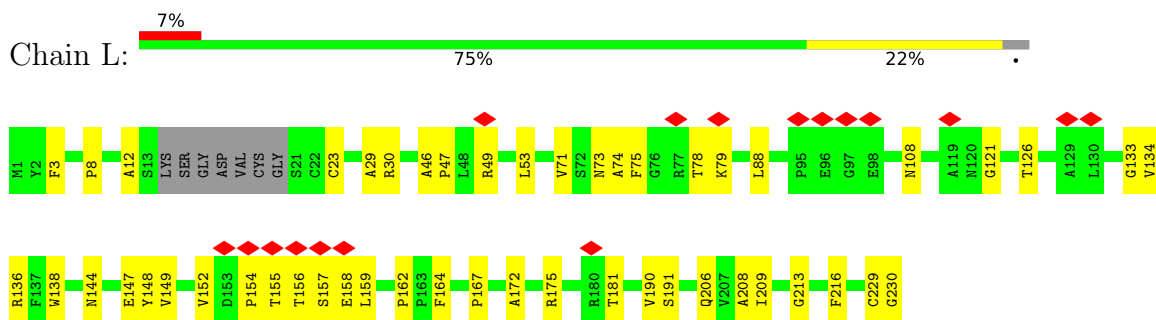
- Molecule 1: Collar sheath protein, gp13



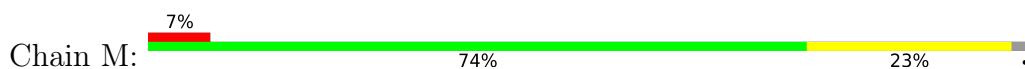
- Molecule 1: Collar sheath protein, gp13

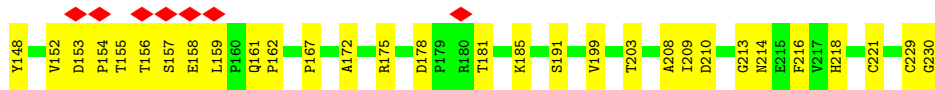


- Molecule 1: Collar sheath protein, gp13

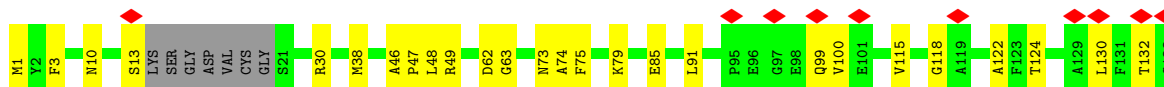
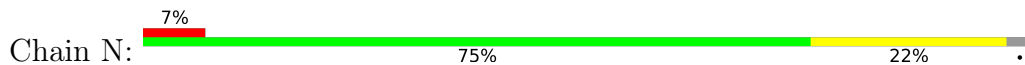


- Molecule 1: Collar sheath protein, gp13





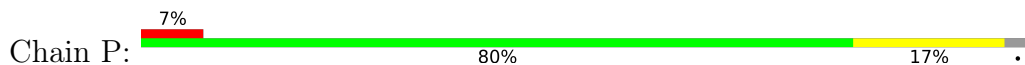
• Molecule 1: Collar sheath protein, gp13



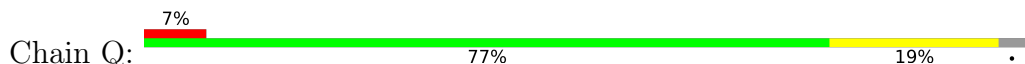
• Molecule 1: Collar sheath protein, gp13

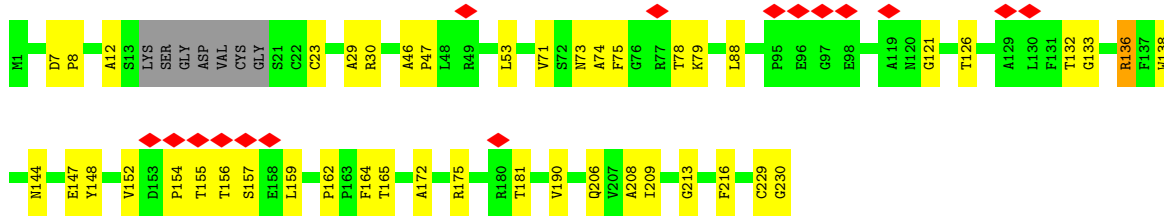


• Molecule 1: Collar sheath protein, gp13

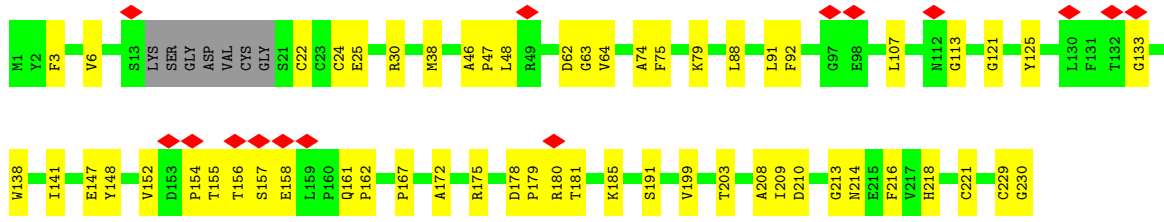
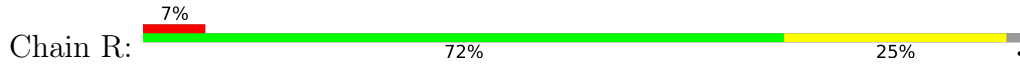


• Molecule 1: Collar sheath protein, gp13

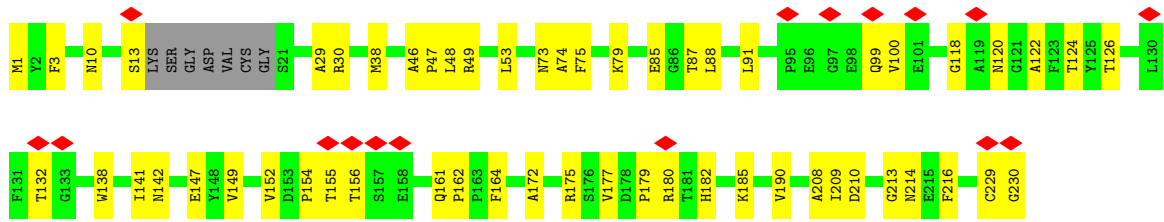
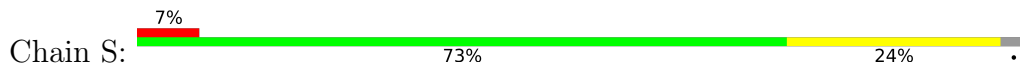




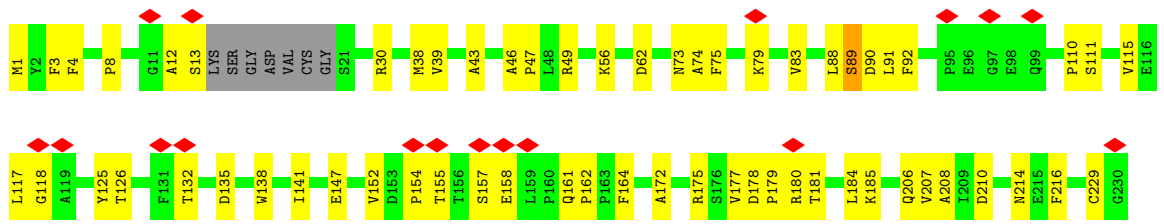
• Molecule 1: Collar sheath protein, gp13



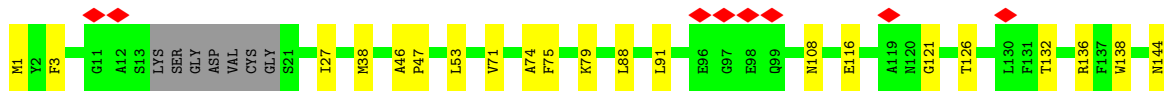
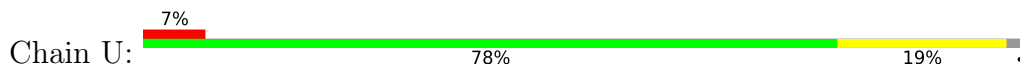
• Molecule 1: Collar sheath protein, gp13



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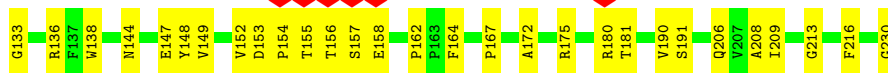
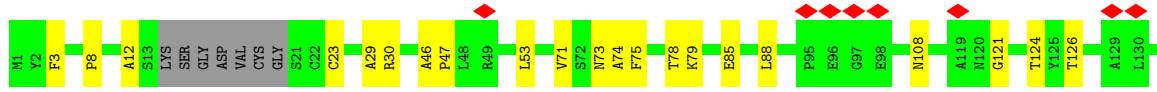
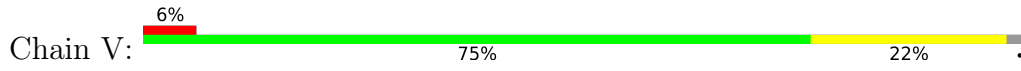


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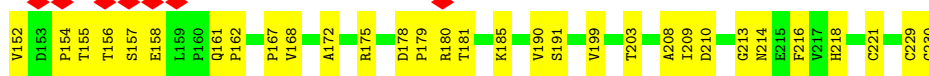
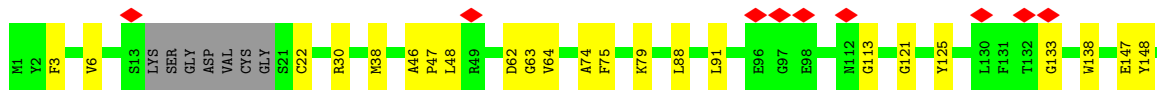
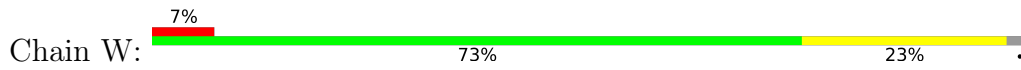




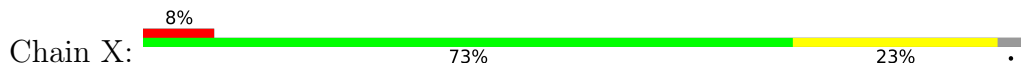
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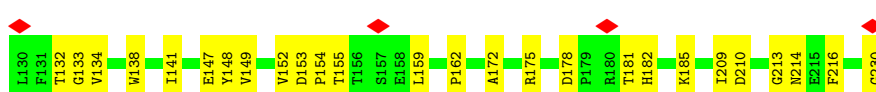
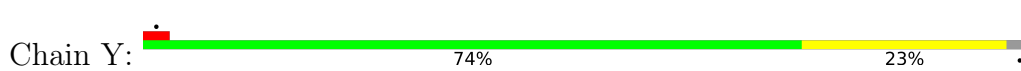
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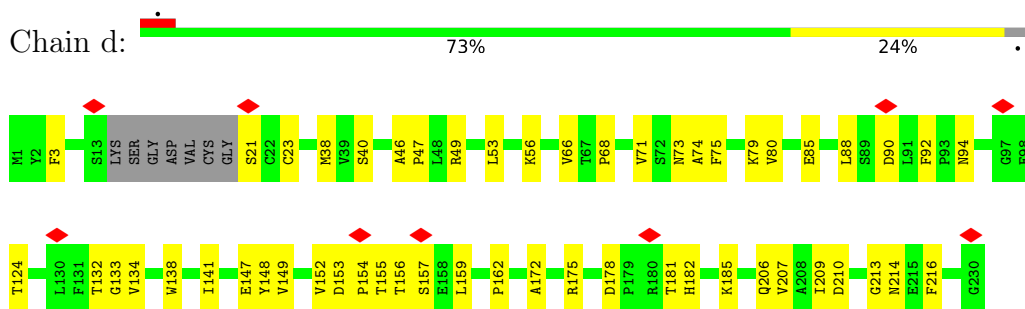
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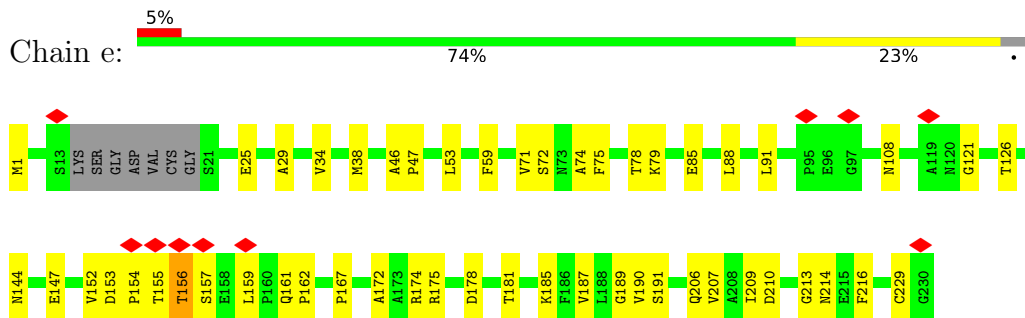
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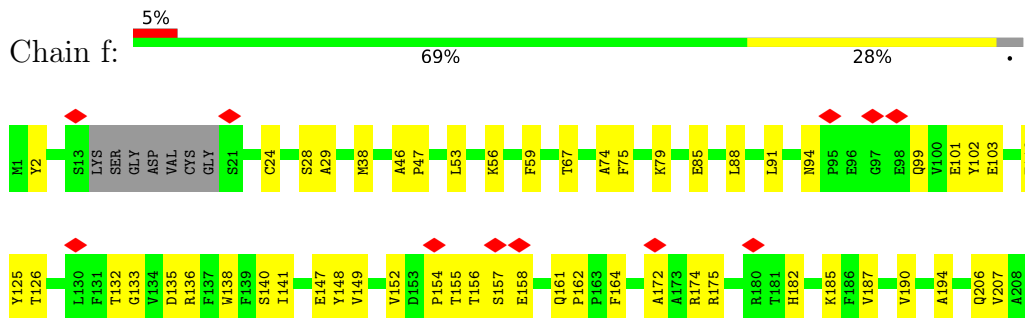
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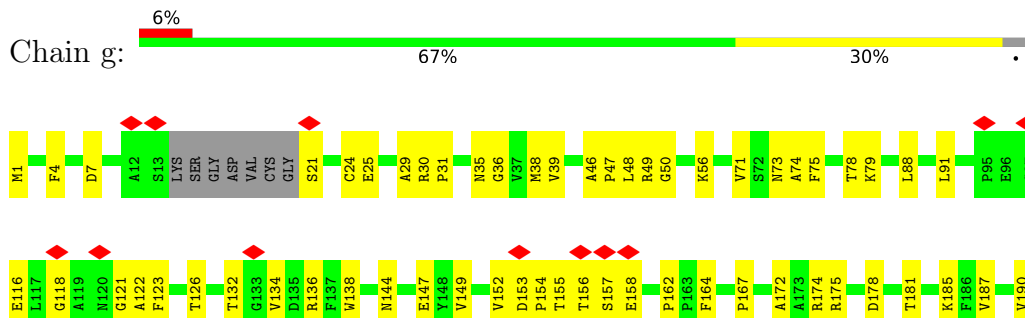
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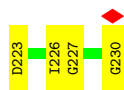


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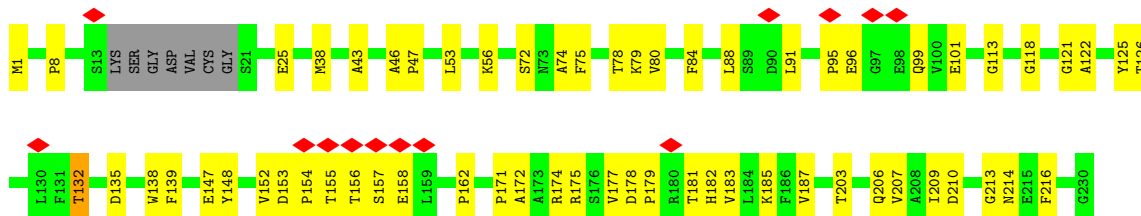


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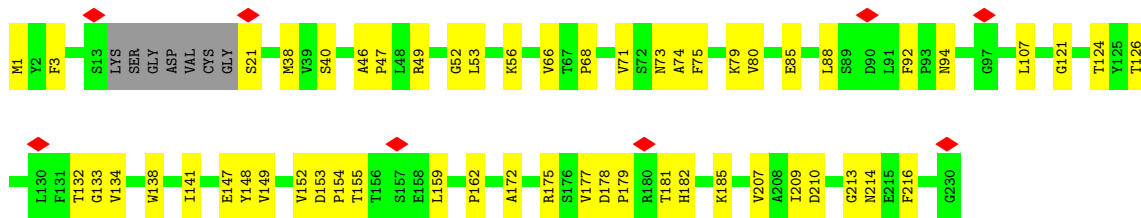




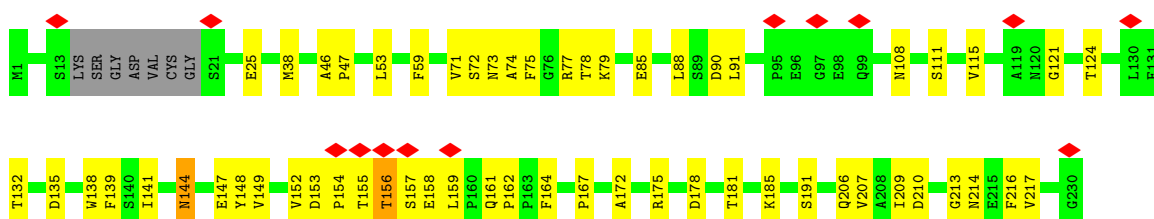
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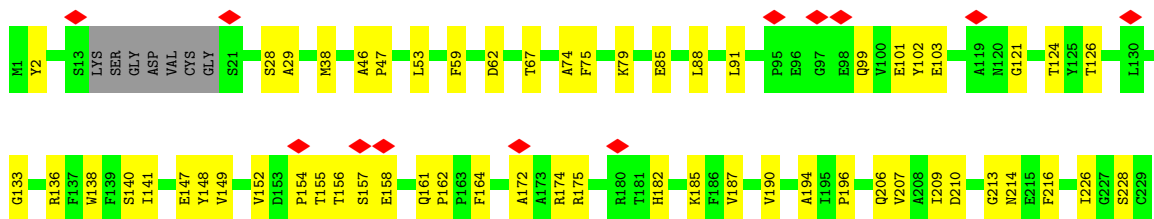
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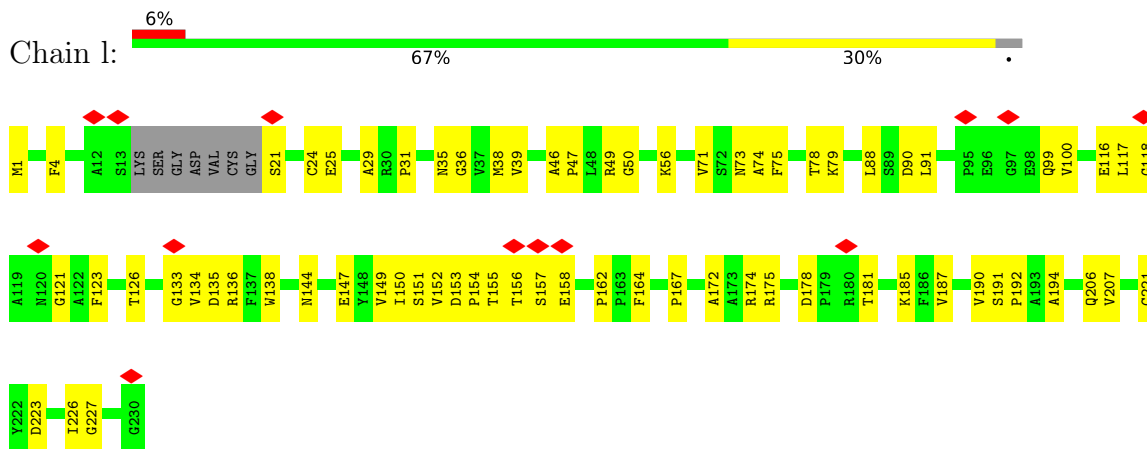
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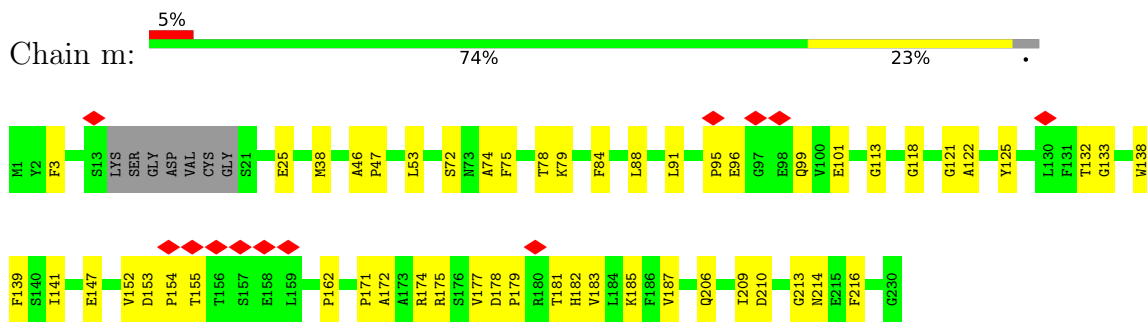
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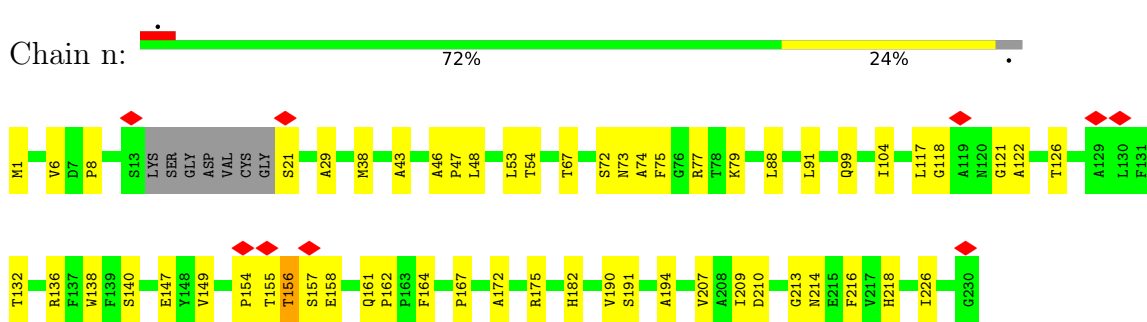
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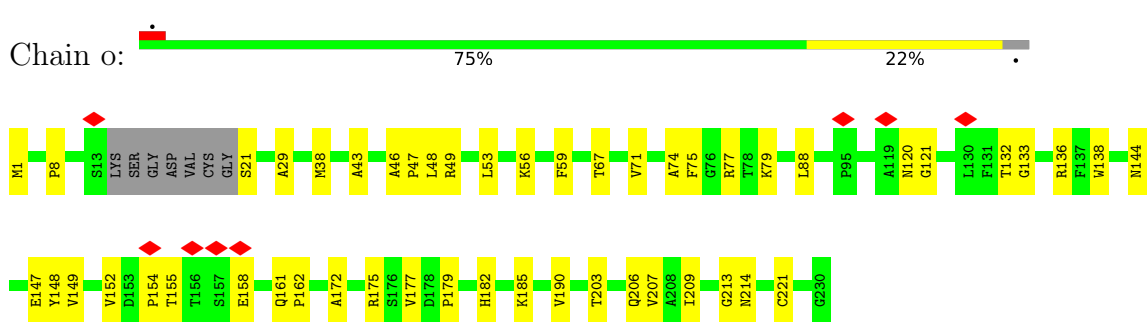
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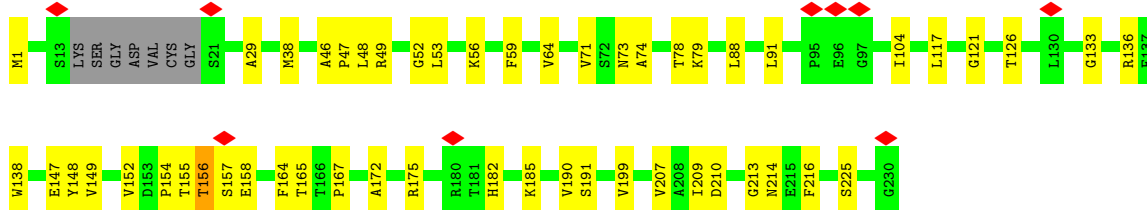


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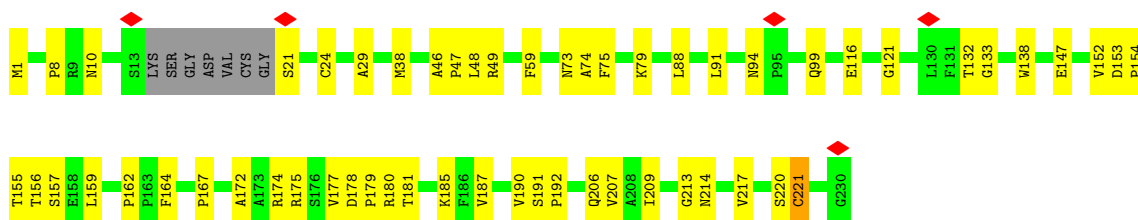
• Molecule 1: Collar sheath protein, gp13

Chain p:  74% 22%



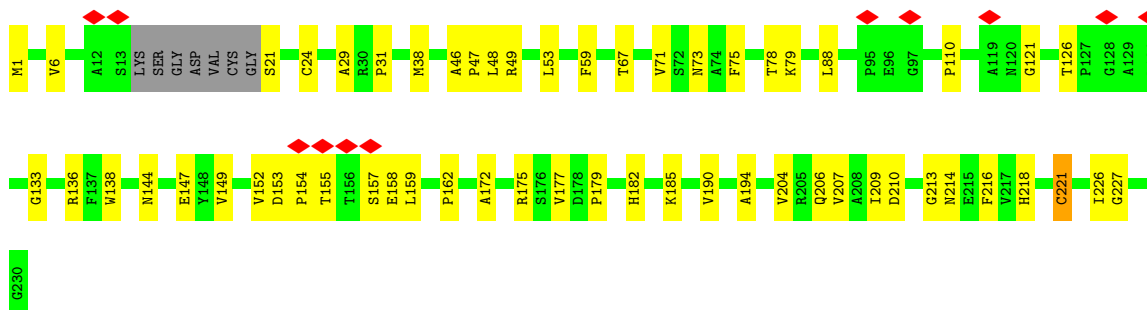
- Molecule 1: Collar sheath protein, gp13

Chain q:  72% 24%



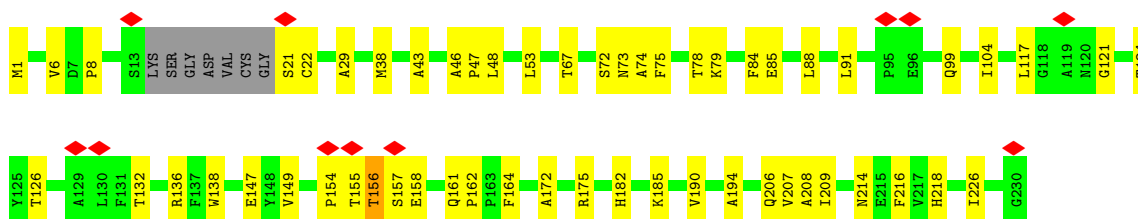
- Molecule 1: Collar sheath protein, gp13

Chain r:  5% 72% 24%




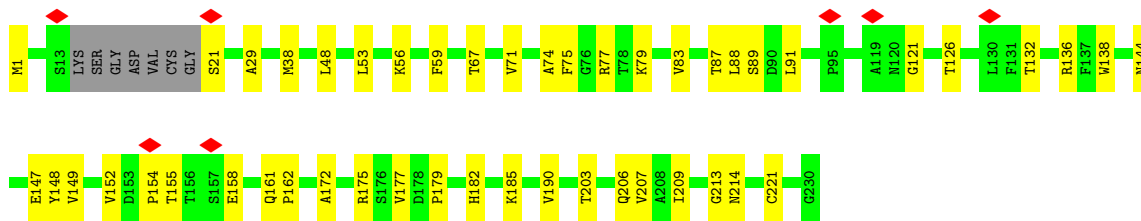
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Chain s:  5% 73% 24%

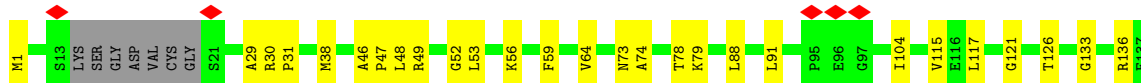


- Molecule 1: Collar sheath protein, gp13

Chain t:  76% 21%



• Molecule 1: Collar sheath protein, gp13



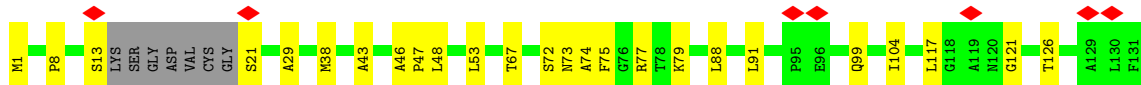
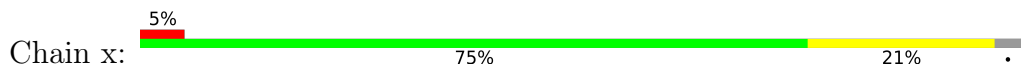
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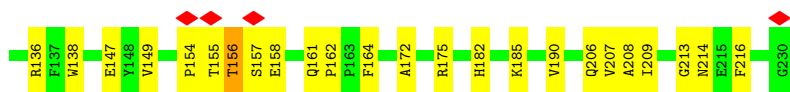


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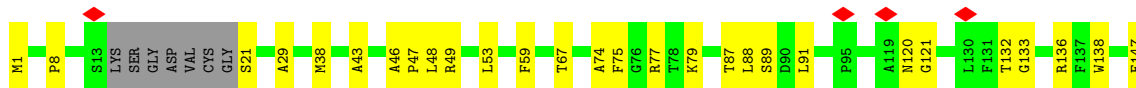
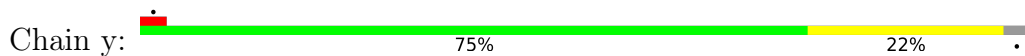


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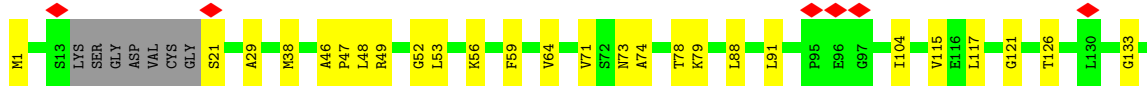




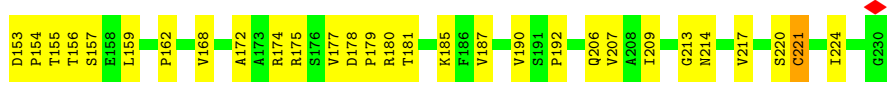
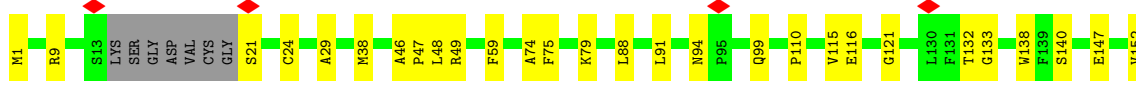
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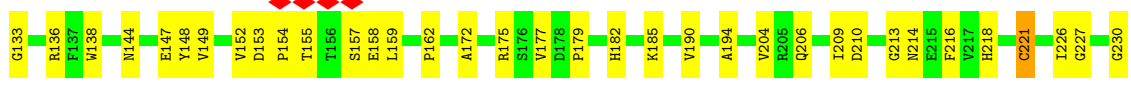
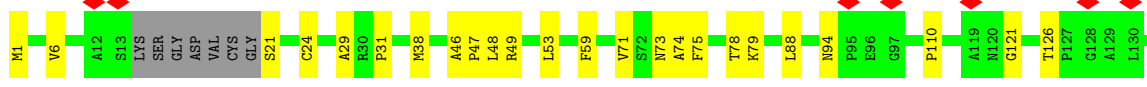
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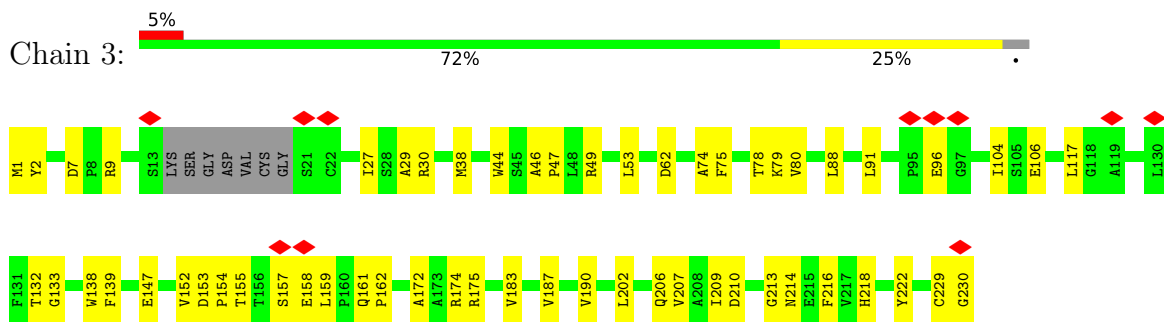
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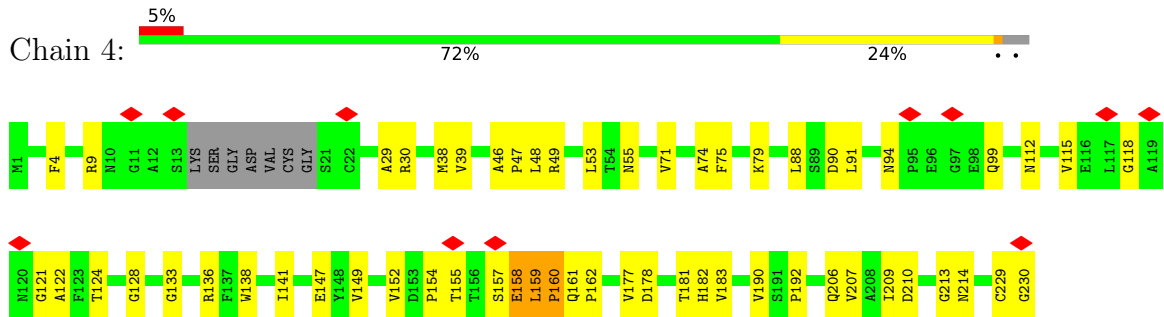
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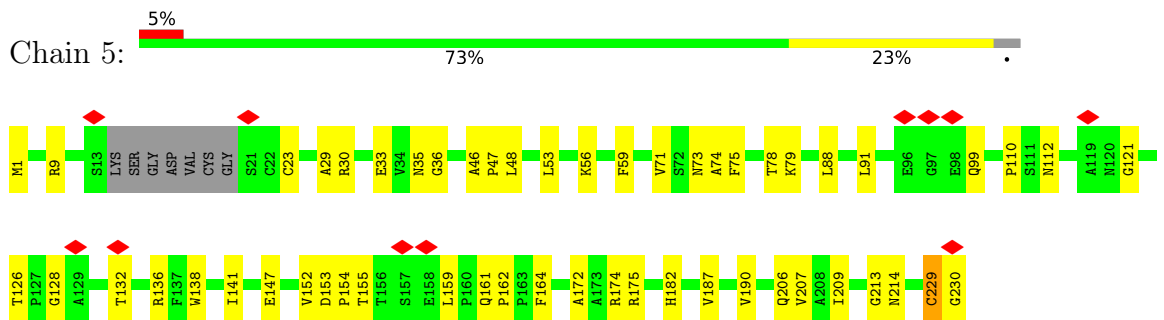
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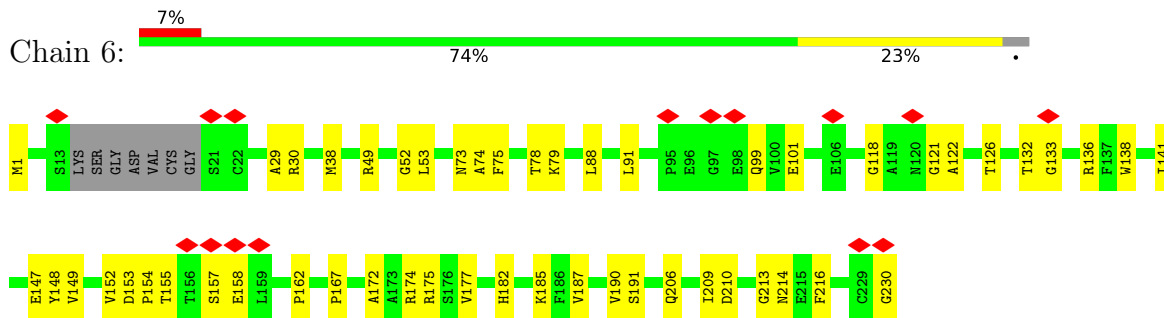
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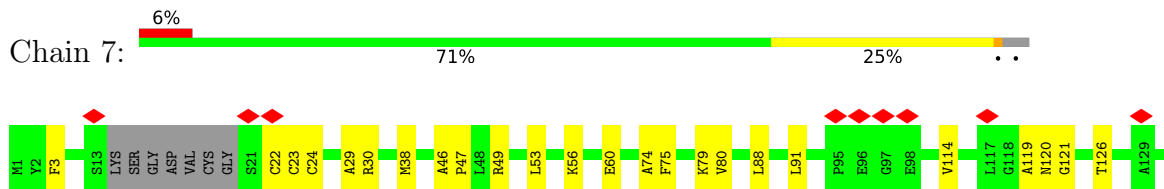
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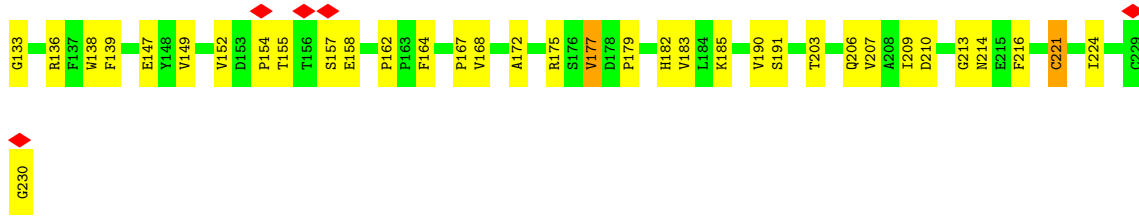


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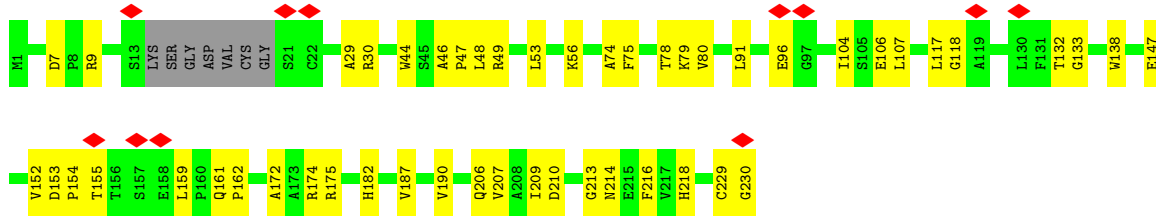
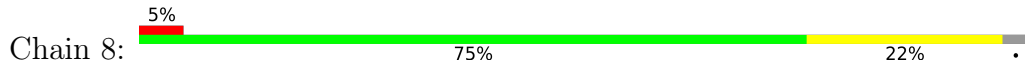


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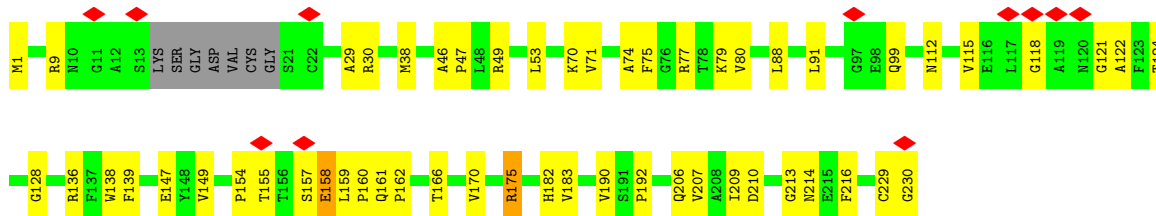
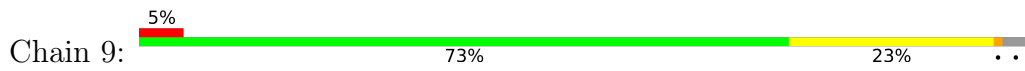




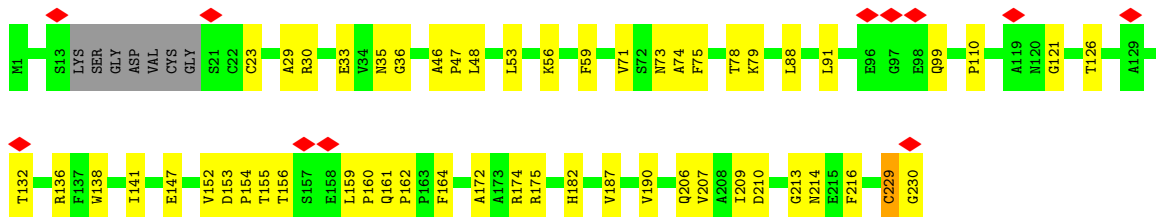
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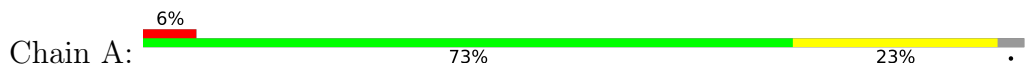
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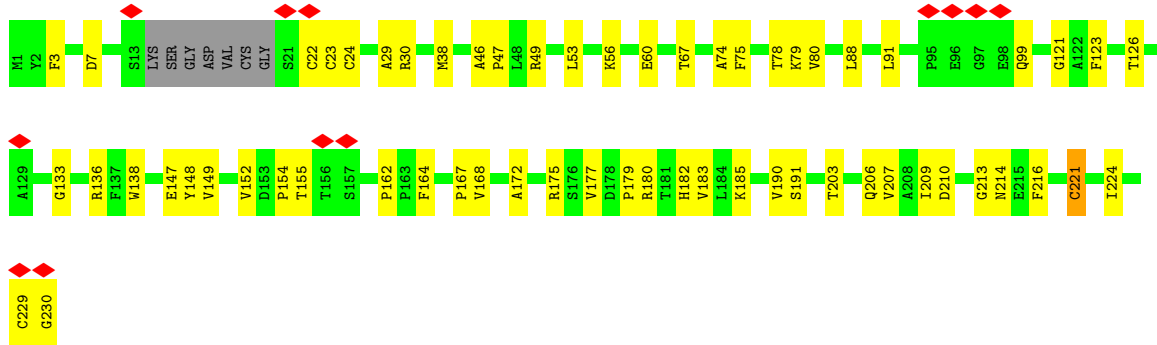


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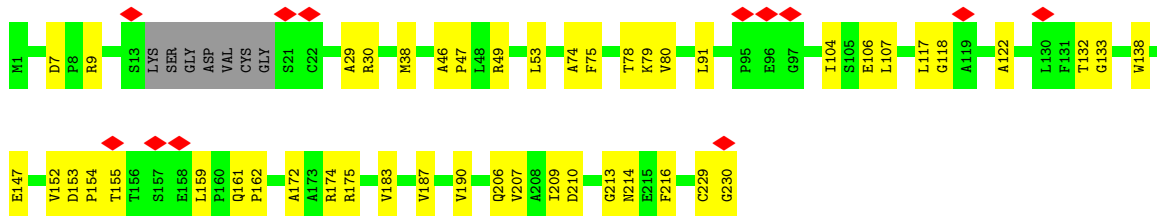
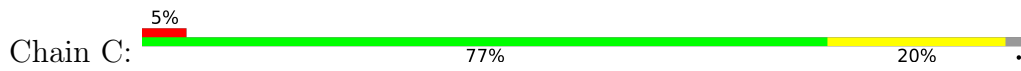




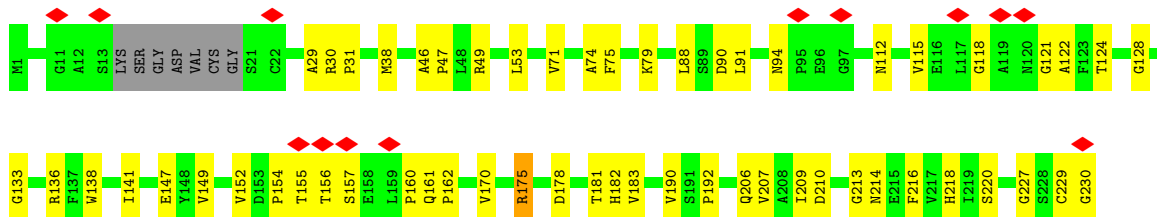
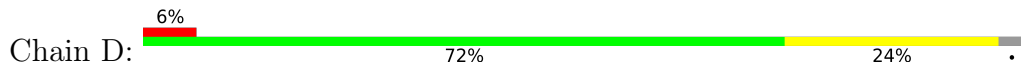
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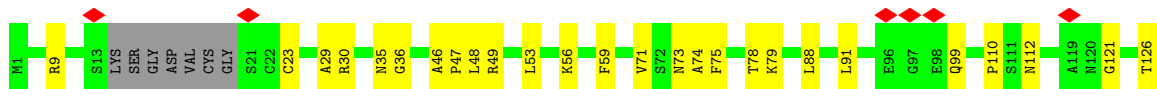
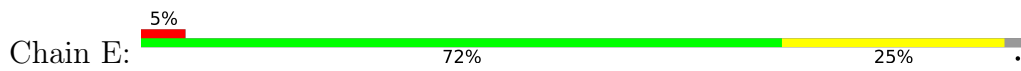
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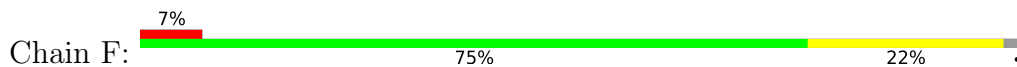


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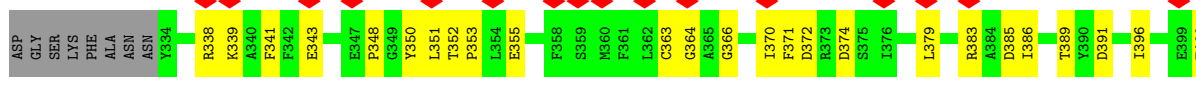
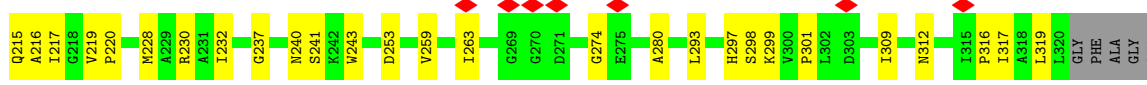
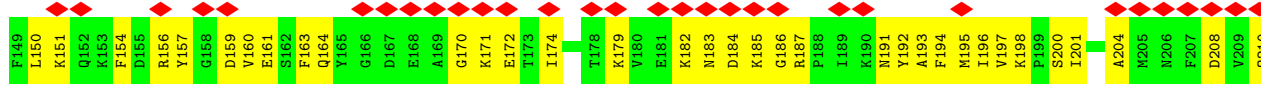
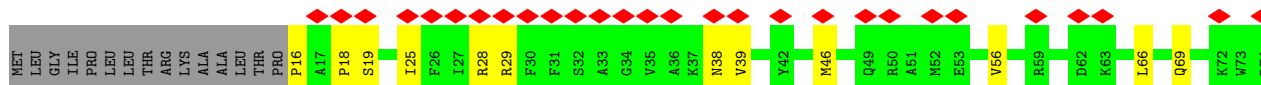
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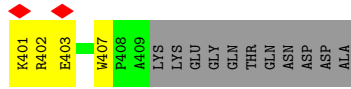


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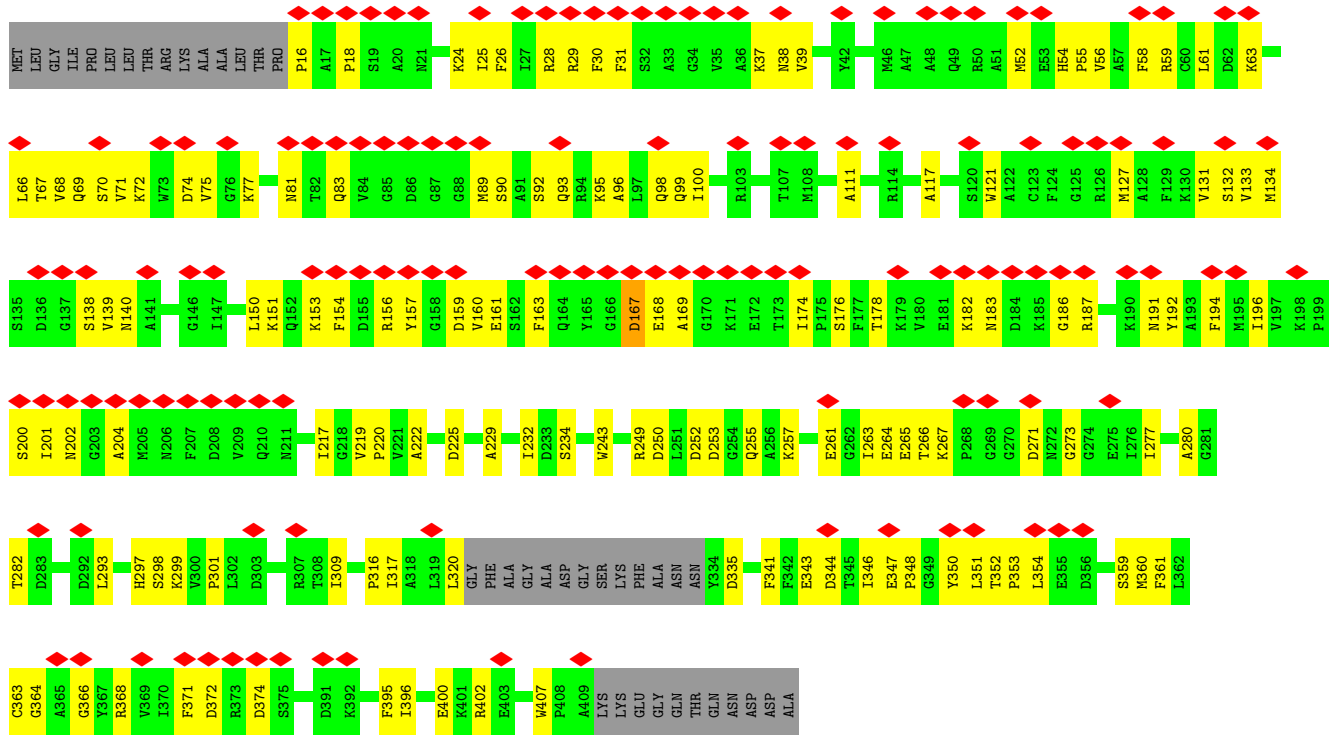


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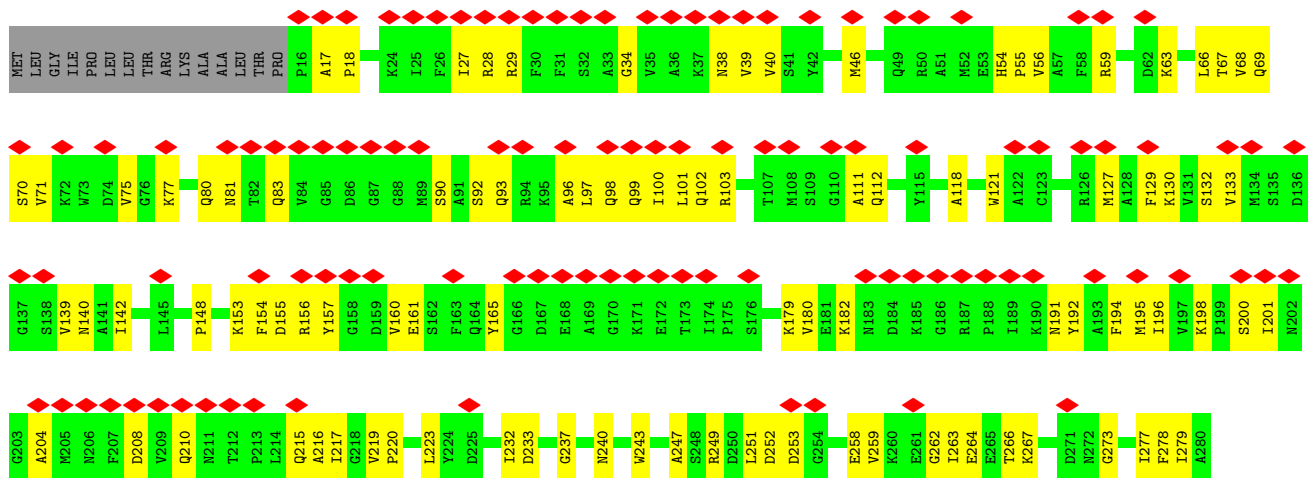


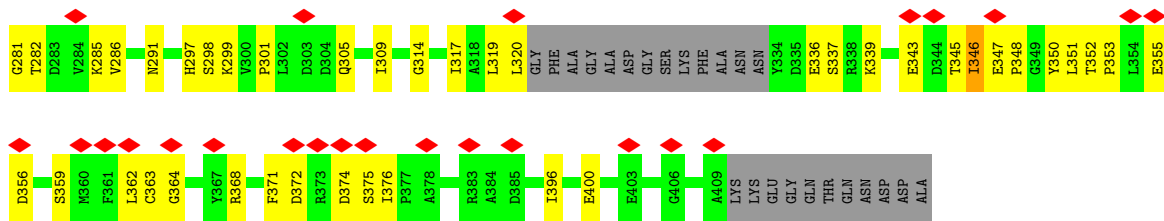


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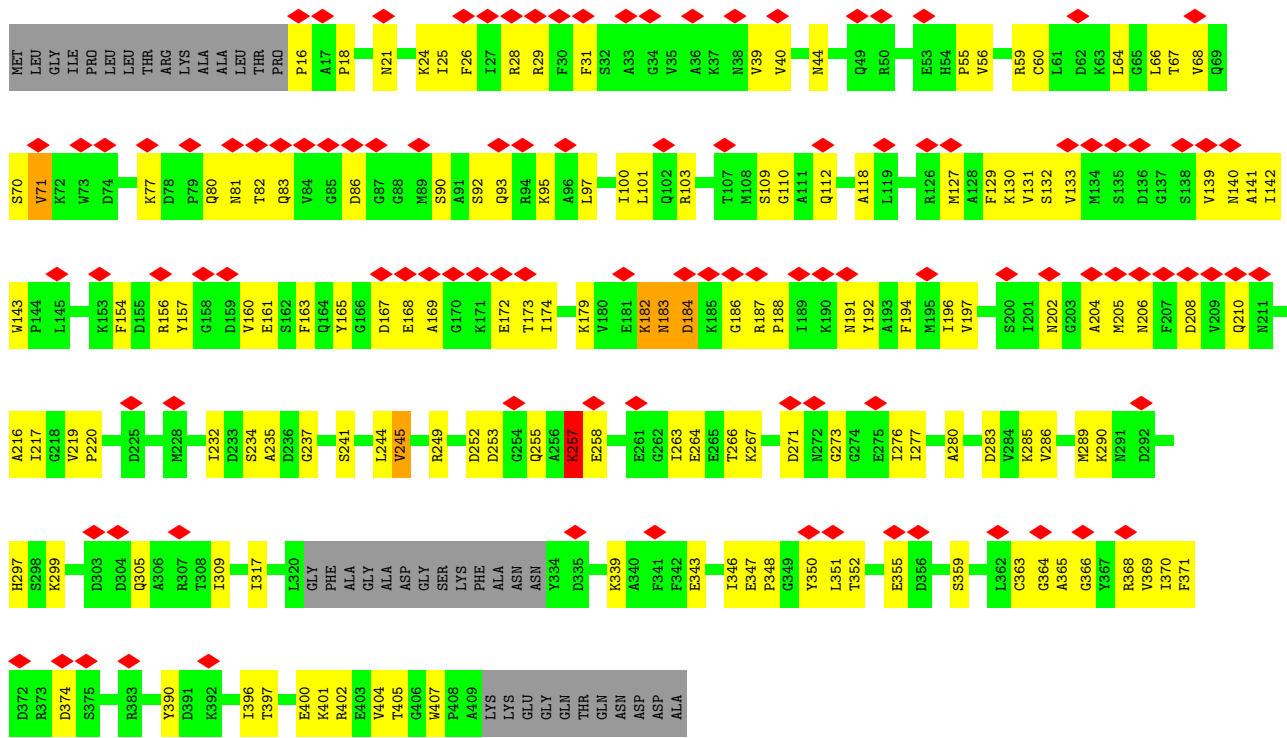


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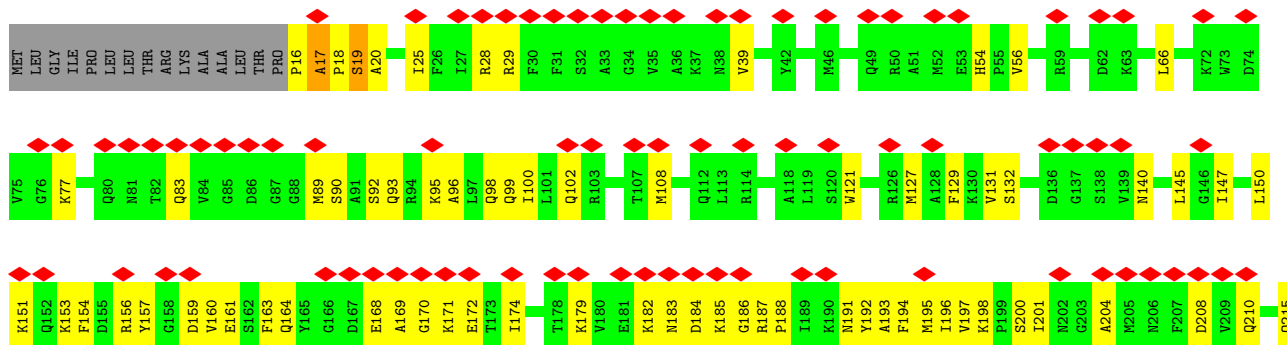


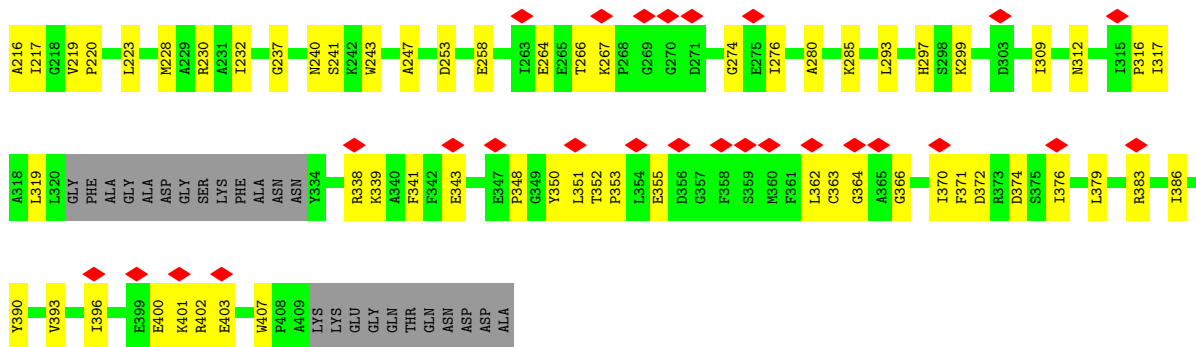


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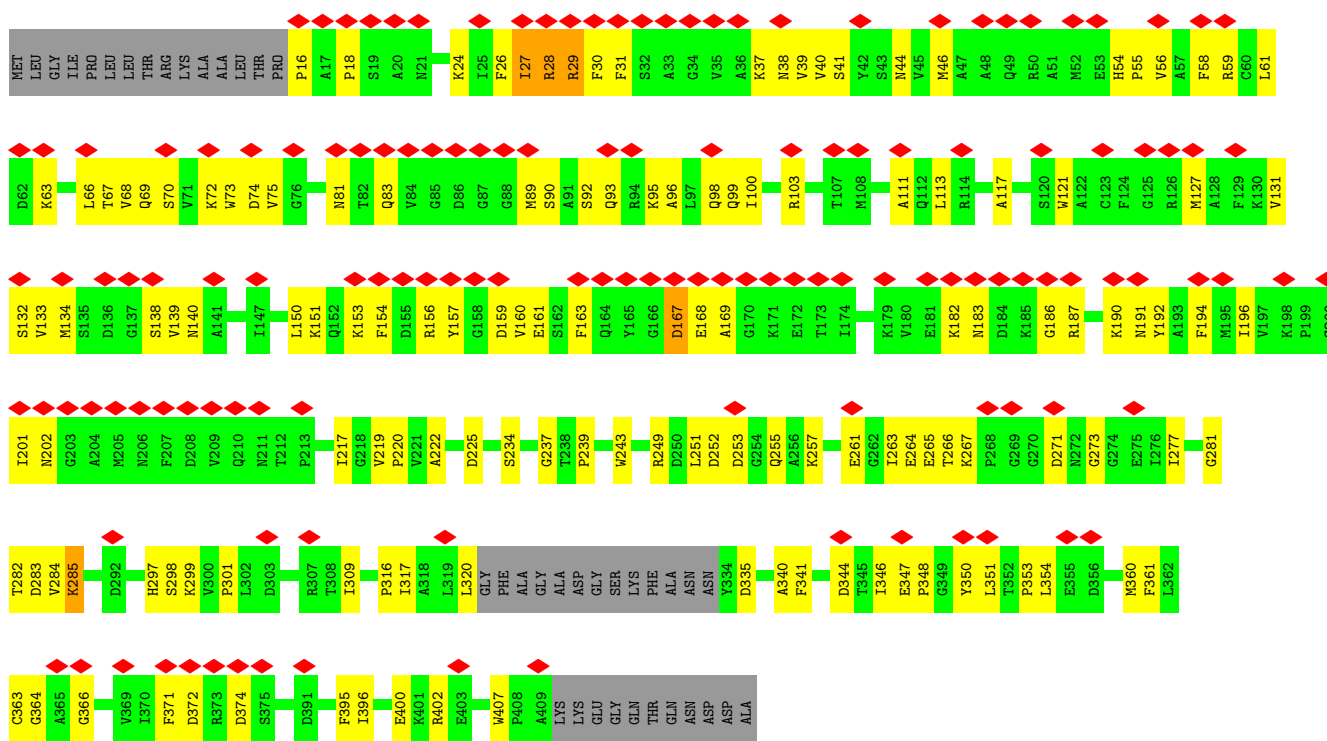


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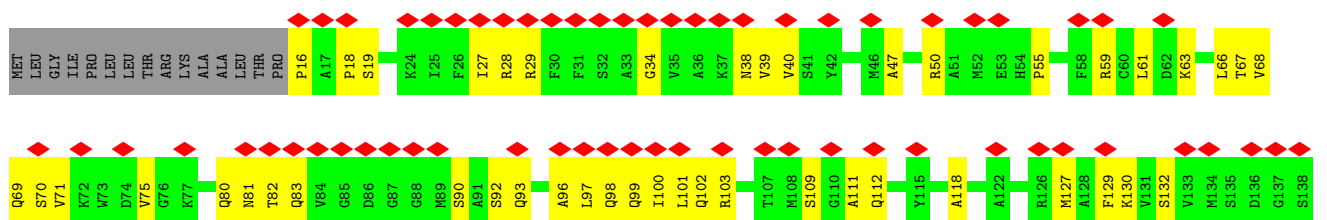


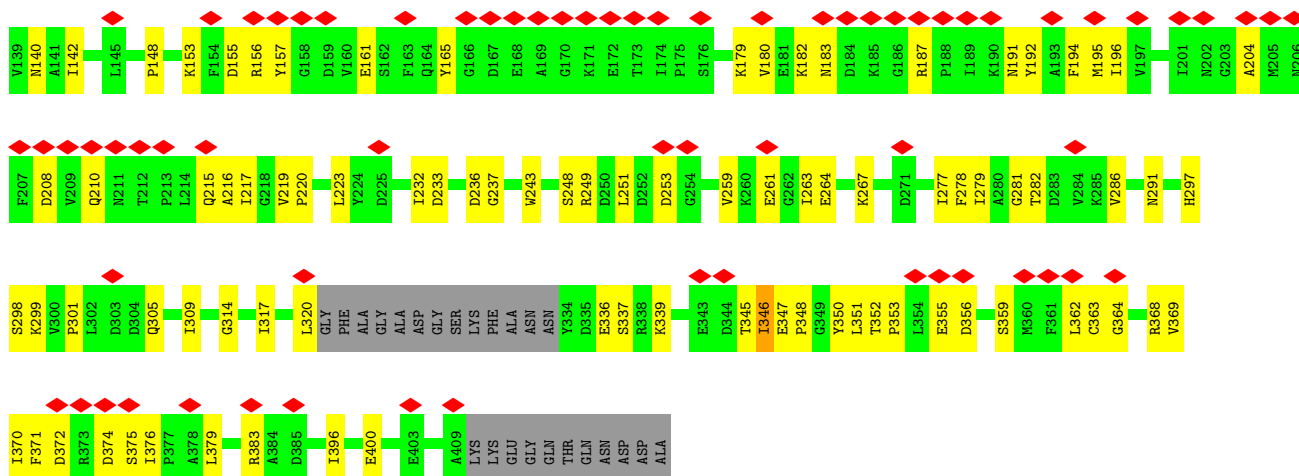


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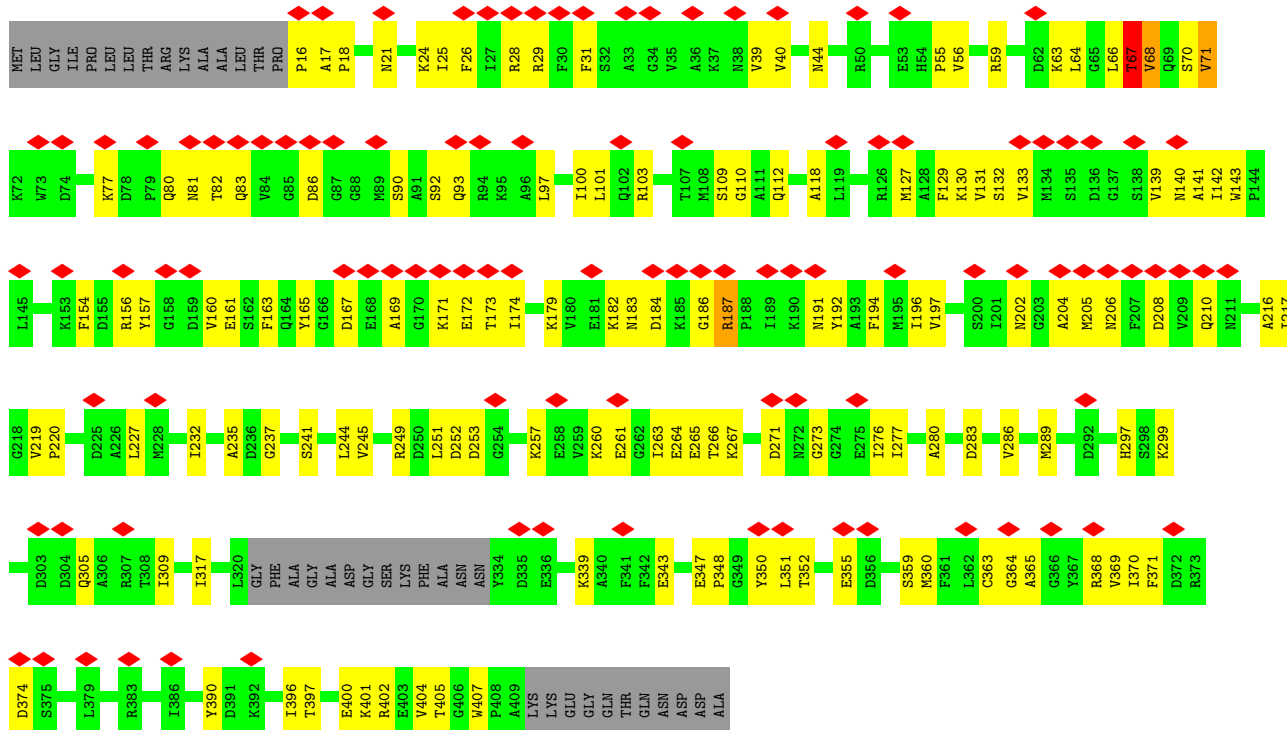


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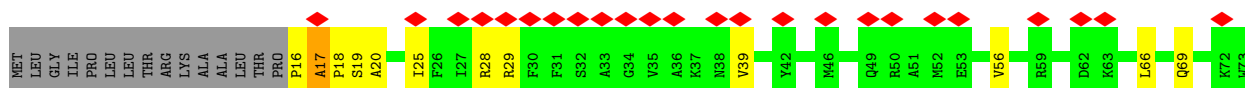




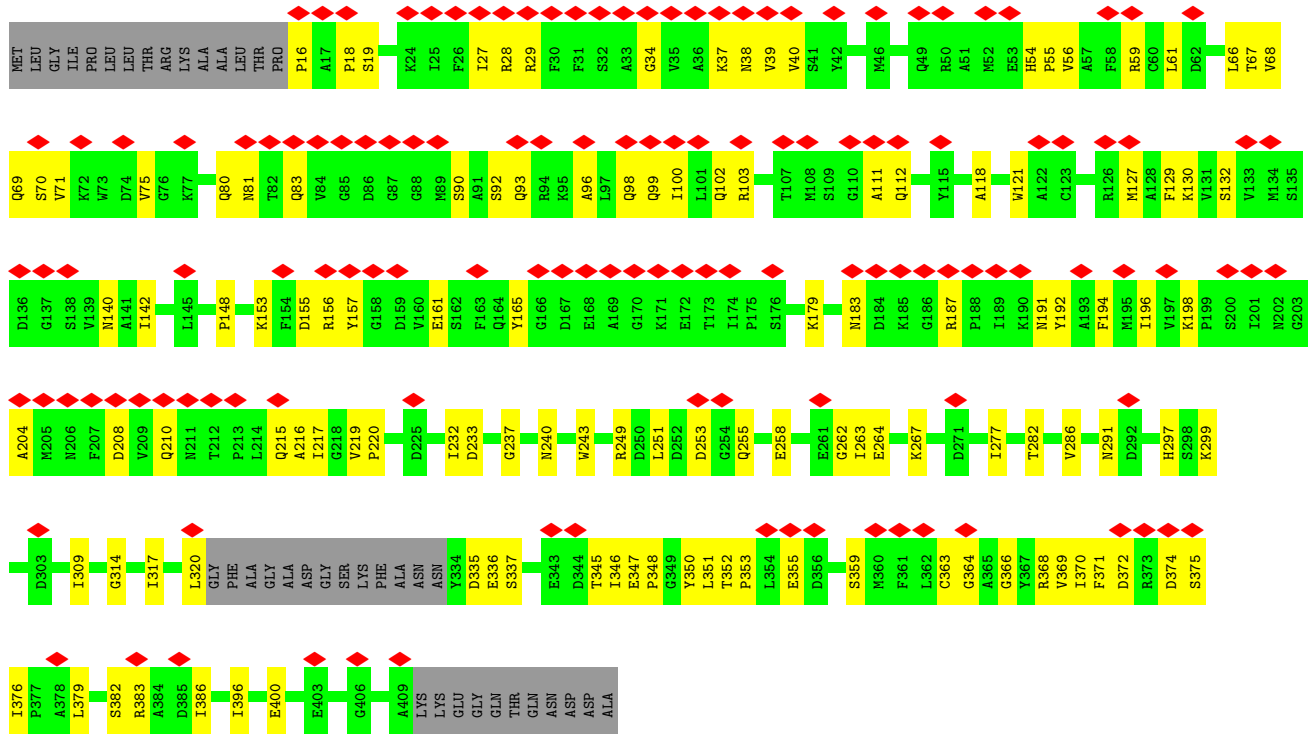
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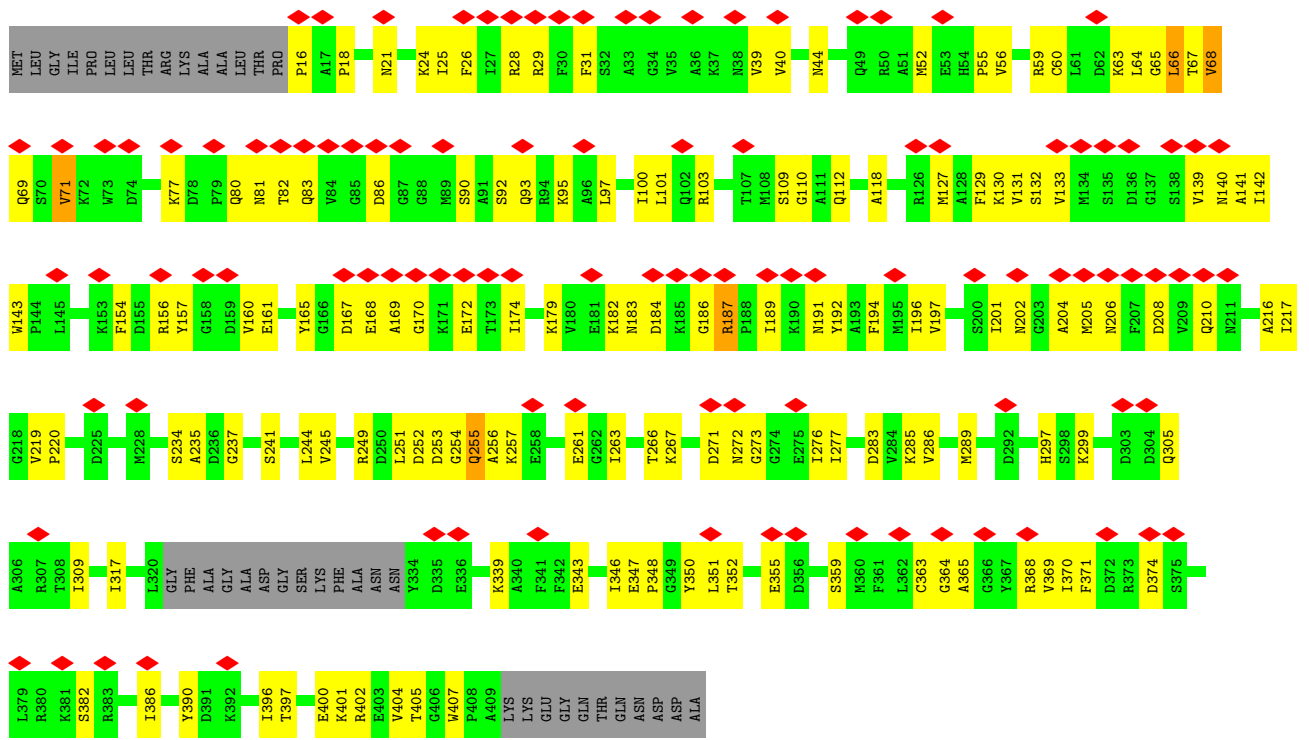
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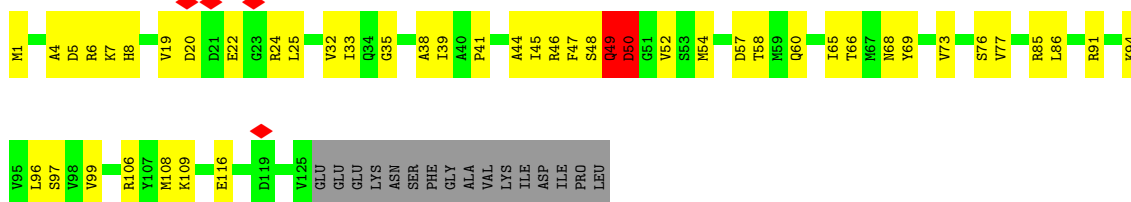
• Molecule 2: Portal protein, gp7



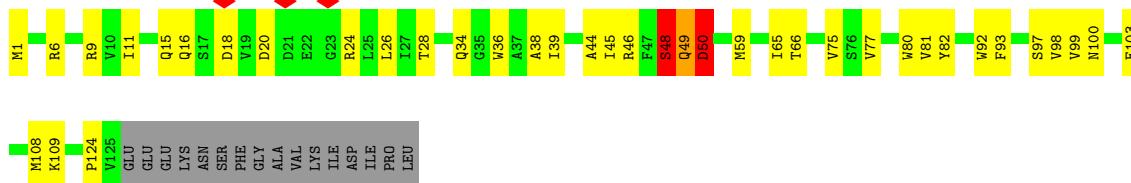
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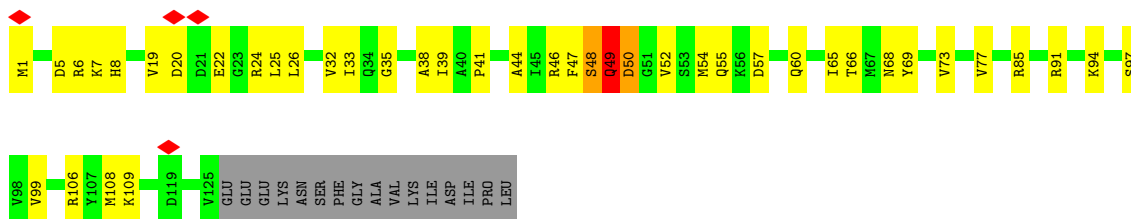
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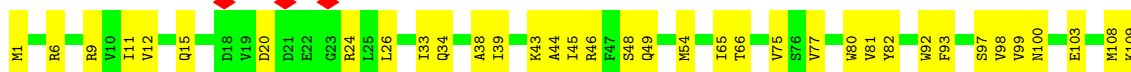
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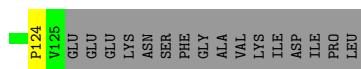


• Molecule 3: Neck 2 protein, gp15

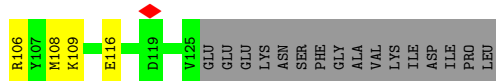
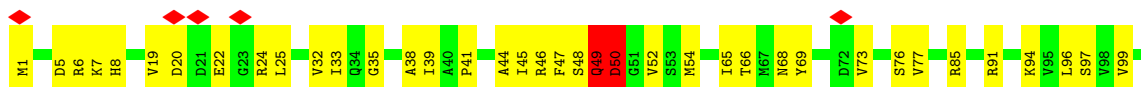


• Molecule 3: Neck 2 protein, gp15

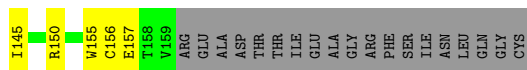




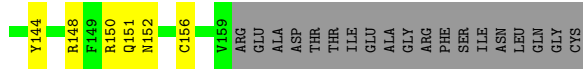
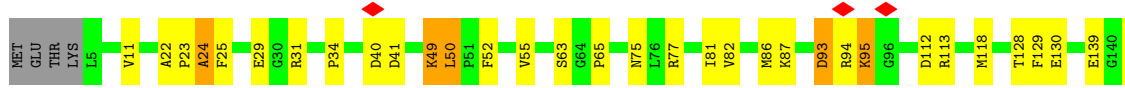
• Molecule 3: Neck 2 protein, gp15



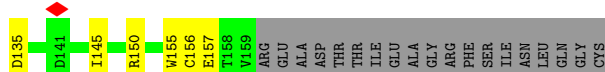
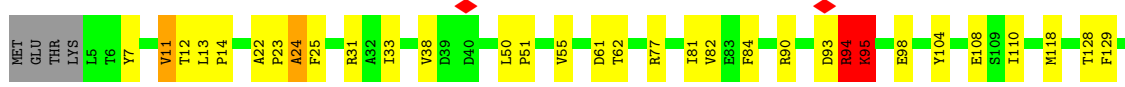
• Molecule 4: Tail-terminator protein, gp18



• Molecule 4: Tail-terminator protein, gp18

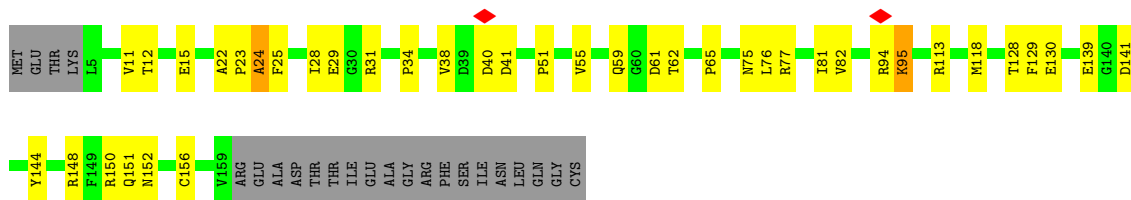


• Molecule 4: Tail-terminator protein, gp18

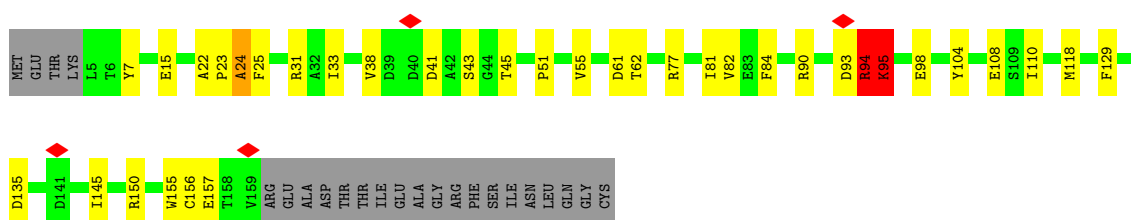


• Molecule 4: Tail-terminator protein, gp18

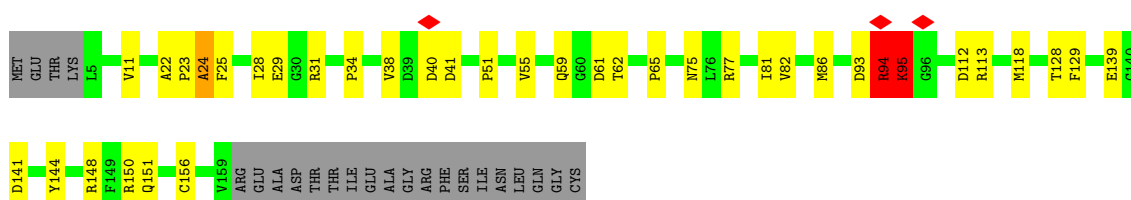




• Molecule 4: Tail-terminator protein, gp18



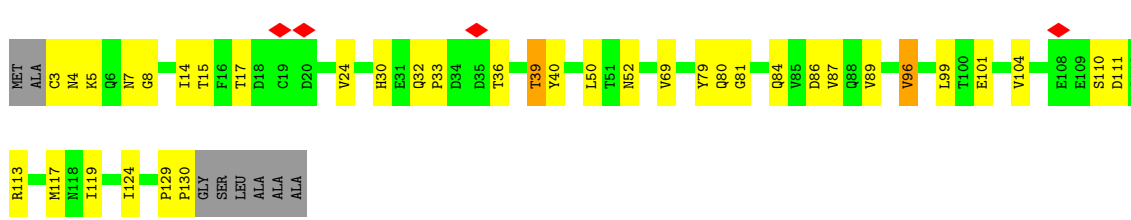
• Molecule 4: Tail-terminator protein, gp18



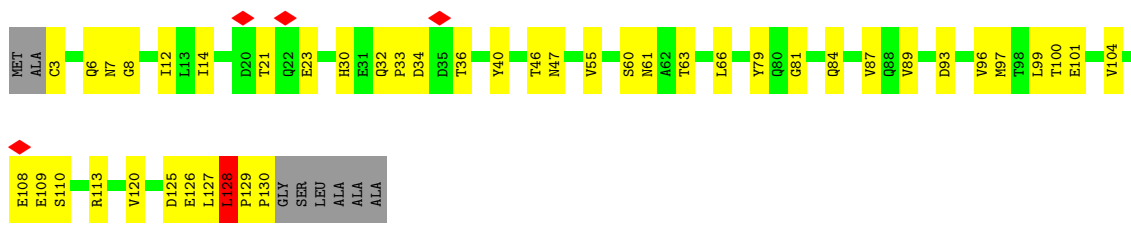
• Molecule 5: Tail-tube, gp21



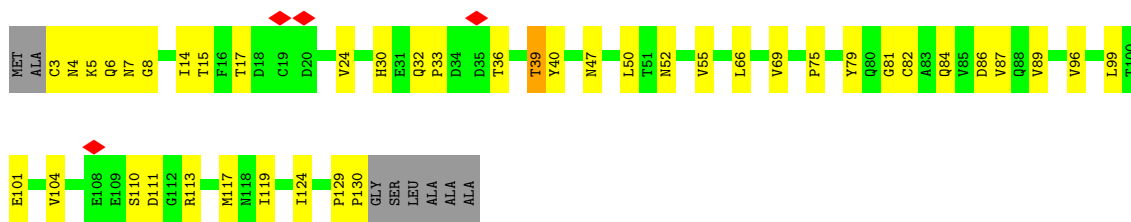
• Molecule 5: Tail-tube, gp21



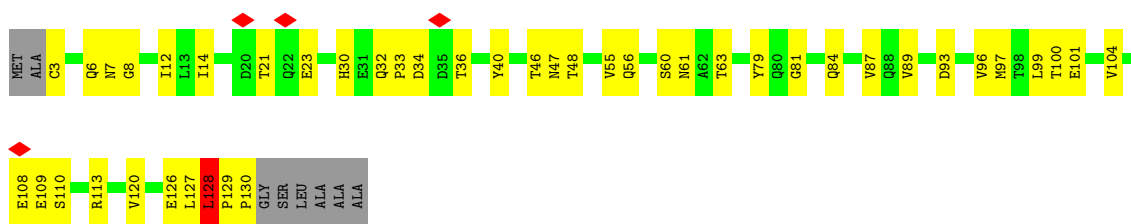
• Molecule 5: Tail-tube, gp21



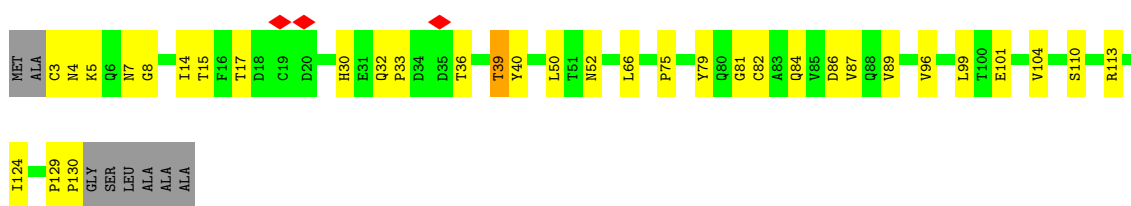
• Molecule 5: Tail-tube, gp21



• Molecule 5: Tail-tube, gp21



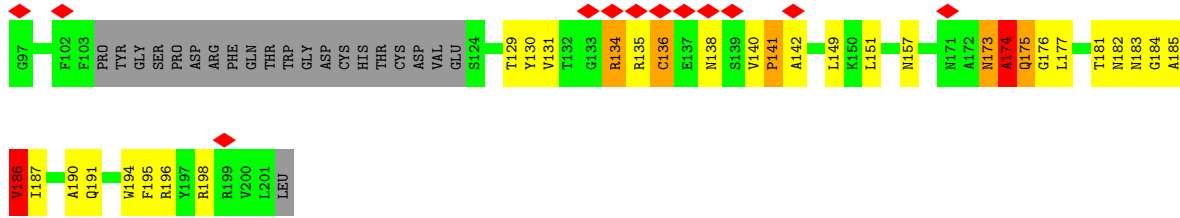
• Molecule 5: Tail-tube, gp21



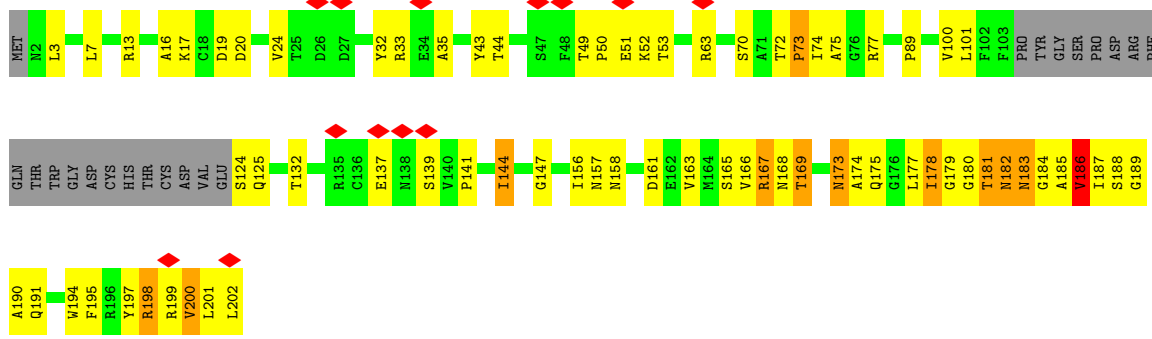
• Molecule 6: Neck 1 protein, gp14



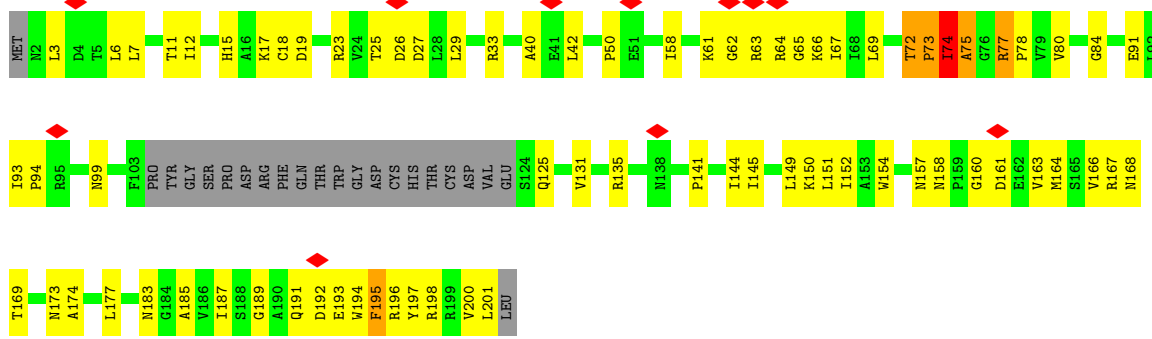




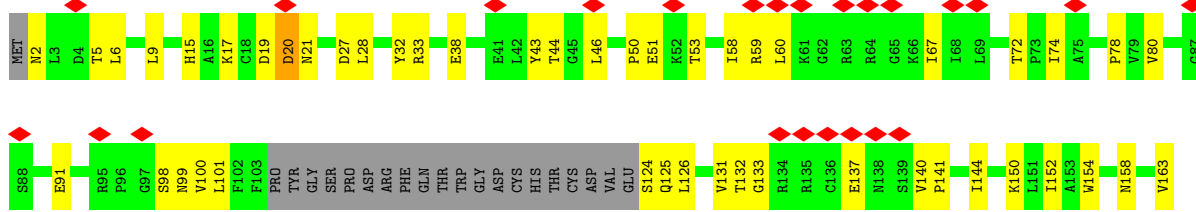
• Molecule 6: Neck 1 protein, gp14



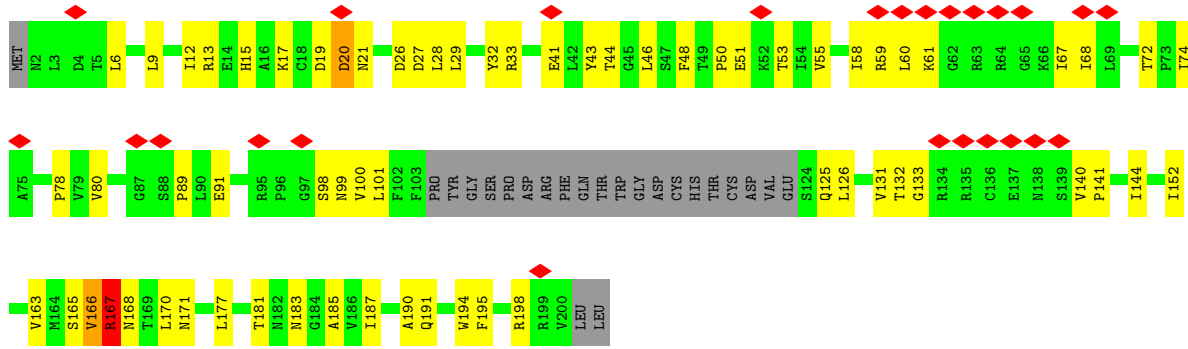
• Molecule 6: Neck 1 protein, gp14



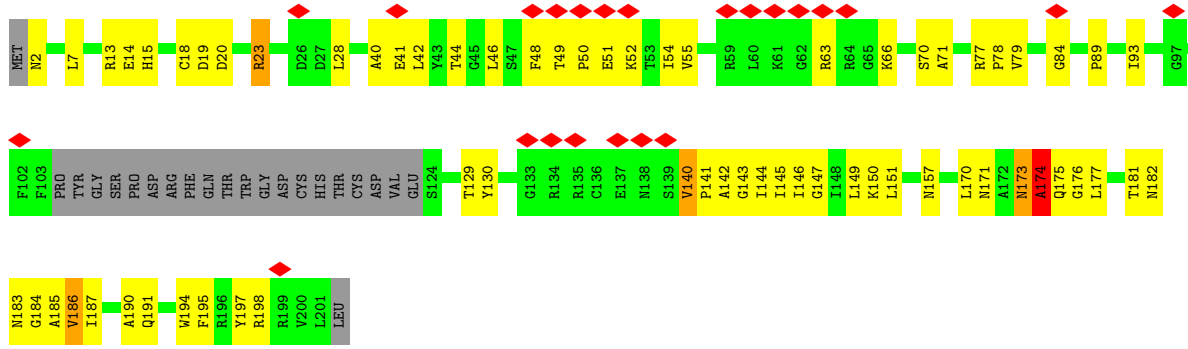
• Molecule 6: Neck 1 protein, gp14







• Molecule 6: Neck 1 protein, gp14



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10216	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.780	Depositor
Minimum map value	-0.421	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.15	Depositor
Map size ( $\text{\AA}$ )	483.84003, 483.84003, 483.84003	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.08, 1.08, 1.08	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	0	0.35	0/1723	0.49	0/2353
1	1	0.39	0/1723	0.52	0/2353
1	2	0.40	0/1723	0.51	0/2353
1	3	0.33	0/1723	0.48	0/2353
1	4	0.34	0/1723	0.47	0/2353
1	5	0.35	0/1723	0.49	0/2353
1	6	0.33	0/1723	0.48	0/2353
1	7	0.34	0/1723	0.51	0/2353
1	8	0.33	0/1723	0.48	0/2353
1	9	0.35	0/1723	0.48	0/2353
1	A	0.33	0/1723	0.50	0/2353
1	B	0.34	0/1723	0.51	0/2353
1	C	0.33	0/1723	0.49	0/2353
1	D	0.34	0/1723	0.47	0/2353
1	E	0.35	0/1723	0.48	0/2353
1	F	0.33	0/1723	0.47	0/2353
1	G	0.34	0/1723	0.50	0/2353
1	J	0.38	0/1723	0.51	0/2353
1	K	0.38	0/1723	0.51	0/2353
1	L	0.37	0/1723	0.48	0/2353
1	M	0.36	0/1723	0.49	0/2353
1	N	0.36	0/1723	0.50	0/2353
1	O	0.38	0/1723	0.50	0/2353
1	P	0.38	0/1723	0.52	0/2353
1	Q	0.38	0/1723	0.49	0/2353
1	R	0.35	0/1723	0.50	0/2353
1	S	0.36	0/1723	0.50	0/2353
1	T	0.38	0/1723	0.53	1/2353 (0.0%)
1	U	0.38	0/1723	0.52	0/2353
1	V	0.37	0/1723	0.51	0/2353
1	W	0.35	0/1723	0.50	0/2353
1	X	0.36	0/1723	0.51	0/2353
1	Y	0.39	0/1723	0.50	0/2353
1	Z	0.38	0/1723	0.50	0/2353

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	a	0.39	0/1723	0.50	0/2353
1	b	0.38	0/1723	0.48	0/2353
1	c	0.39	0/1723	0.51	0/2353
1	d	0.39	0/1723	0.50	0/2353
1	e	0.39	0/1723	0.51	0/2353
1	f	0.39	0/1723	0.50	0/2353
1	g	0.38	0/1723	0.48	0/2353
1	h	0.39	0/1723	0.50	0/2353
1	i	0.39	0/1723	0.50	0/2353
1	j	0.39	0/1723	0.50	0/2353
1	k	0.39	0/1723	0.50	0/2353
1	l	0.38	0/1723	0.47	0/2353
1	m	0.39	0/1723	0.51	0/2353
1	n	0.38	0/1723	0.49	0/2353
1	o	0.39	0/1723	0.49	0/2353
1	p	0.38	0/1723	0.50	0/2353
1	q	0.39	0/1723	0.52	0/2353
1	r	0.40	0/1723	0.51	0/2353
1	s	0.39	0/1723	0.50	0/2353
1	t	0.39	0/1723	0.49	0/2353
1	u	0.38	0/1723	0.50	0/2353
1	v	0.39	0/1723	0.53	0/2353
1	w	0.39	0/1723	0.51	0/2353
1	x	0.39	0/1723	0.50	0/2353
1	y	0.39	0/1723	0.49	0/2353
1	z	0.38	0/1723	0.49	0/2353
2	AA	0.31	0/3000	0.49	0/4056
2	AB	0.30	0/3000	0.54	2/4056 (0.0%)
2	AC	0.29	0/3000	0.50	0/4056
2	AD	0.31	0/3000	0.53	1/4056 (0.0%)
2	AE	0.30	0/3000	0.51	0/4056
2	AF	0.30	0/3000	0.54	4/4056 (0.1%)
2	AG	0.29	0/3000	0.50	0/4056
2	AH	0.30	0/3000	0.52	0/4056
2	AI	0.31	0/3000	0.48	0/4056
2	AJ	0.29	0/3000	0.55	4/4056 (0.1%)
2	AK	0.29	0/3000	0.51	0/4056
2	AL	0.31	0/3000	0.53	1/4056 (0.0%)
3	AM	0.36	0/1017	0.46	0/1381
3	AN	0.38	0/1017	0.46	0/1381
3	AO	0.36	0/1017	0.46	0/1381
3	AP	0.39	0/1017	0.51	1/1381 (0.1%)
3	H	0.39	0/1017	0.48	0/1381

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	I	0.38	0/1017	0.51	1/1381 (0.1%)
4	AQ	0.39	0/1281	0.46	0/1734
4	AR	0.41	0/1281	0.48	0/1734
4	AS	0.39	0/1281	0.50	1/1734 (0.1%)
4	AT	0.38	0/1281	0.46	0/1734
4	AW	0.39	0/1281	0.48	1/1734 (0.1%)
4	AX	0.41	0/1281	0.47	1/1734 (0.1%)
5	AU	0.41	0/993	0.48	0/1358
5	AV	0.40	0/993	0.47	0/1358
5	AY	0.40	0/993	0.46	0/1358
5	AZ	0.37	0/993	0.44	0/1358
5	Aa	0.36	0/993	0.44	0/1358
5	Ab	0.37	0/993	0.44	0/1358
6	R3	0.45	0/1420	0.57	0/1927
6	R4	0.49	1/1420 (0.1%)	0.59	0/1927
6	R5	0.46	0/1420	0.60	2/1927 (0.1%)
6	S3	0.43	0/1412	0.61	0/1916
6	S4	0.44	0/1412	0.60	1/1916 (0.1%)
6	S5	0.44	0/1412	0.61	1/1916 (0.1%)
6	T3	0.37	0/1404	0.55	0/1905
6	T4	0.38	0/1404	0.57	1/1905 (0.1%)
6	T5	0.37	0/1404	0.55	0/1905
6	U3	0.48	0/1412	0.71	5/1916 (0.3%)
6	U4	0.62	0/1412	0.80	4/1916 (0.2%)
6	U5	0.50	0/1412	0.68	4/1916 (0.2%)
All	All	0.37	1/176070 (0.0%)	0.51	36/239682 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R4	181	THR	CA-C	-6.41	1.49	1.52

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	U4	42	LEU	N-CA-C	-7.76	104.70	114.56
6	U3	42	LEU	N-CA-C	-7.66	104.84	114.56
6	U5	42	LEU	N-CA-C	-7.56	104.96	114.56
2	AJ	167	ASP	CA-C-N	-7.27	110.43	122.79
2	AJ	167	ASP	C-N-CA	-7.27	110.43	122.79

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1679	0	1610	42	0
1	1	1679	0	1609	41	0
1	2	1679	0	1609	41	0
1	3	1679	0	1610	40	0
1	4	1679	0	1610	42	0
1	5	1679	0	1610	41	0
1	6	1679	0	1610	39	0
1	7	1679	0	1610	41	0
1	8	1679	0	1610	40	0
1	9	1679	0	1610	41	0
1	A	1679	0	1610	39	0
1	B	1679	0	1610	46	0
1	C	1679	0	1610	36	0
1	D	1679	0	1610	42	0
1	E	1679	0	1610	47	0
1	F	1679	0	1610	38	0
1	G	1679	0	1610	45	0
1	J	1679	0	1610	45	0
1	K	1679	0	1610	29	0
1	L	1679	0	1610	35	0
1	M	1679	0	1610	35	0
1	N	1679	0	1610	39	0
1	O	1679	0	1610	47	0
1	P	1679	0	1610	26	0
1	Q	1679	0	1610	31	0
1	R	1679	0	1610	39	0
1	S	1679	0	1610	40	0
1	T	1679	0	1610	47	0
1	U	1679	0	1610	28	0
1	V	1679	0	1610	34	0
1	W	1679	0	1610	36	0
1	X	1679	0	1610	39	0
1	Y	1679	0	1609	36	0
1	Z	1679	0	1609	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	1679	0	1609	45	0
1	b	1679	0	1609	45	0
1	c	1679	0	1609	42	0
1	d	1679	0	1609	41	0
1	e	1679	0	1609	38	0
1	f	1679	0	1609	47	0
1	g	1679	0	1609	45	0
1	h	1679	0	1609	47	0
1	i	1679	0	1609	39	0
1	j	1679	0	1609	41	0
1	k	1679	0	1609	42	0
1	l	1679	0	1609	48	0
1	m	1679	0	1609	39	0
1	n	1679	0	1609	41	0
1	o	1679	0	1609	35	0
1	p	1679	0	1609	38	0
1	q	1679	0	1609	40	0
1	r	1679	0	1609	41	0
1	s	1679	0	1609	40	0
1	t	1679	0	1609	33	0
1	u	1679	0	1609	42	0
1	v	1679	0	1609	36	0
1	w	1679	0	1609	40	0
1	x	1679	0	1609	37	0
1	y	1679	0	1609	36	0
1	z	1679	0	1609	41	0
2	AA	2938	0	2906	115	0
2	AB	2938	0	2906	130	0
2	AC	2938	0	2906	156	0
2	AD	2938	0	2906	149	0
2	AE	2938	0	2906	122	0
2	AF	2938	0	2906	136	0
2	AG	2938	0	2906	131	0
2	AH	2938	0	2906	148	0
2	AI	2938	0	2906	121	0
2	AJ	2938	0	2906	130	0
2	AK	2938	0	2906	113	0
2	AL	2938	0	2906	143	0
3	AM	997	0	999	33	0
3	AN	997	0	999	33	0
3	AO	997	0	999	31	0
3	AP	997	0	999	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	997	0	999	41	0
3	I	997	0	999	43	0
4	AQ	1251	0	1189	24	0
4	AR	1251	0	1189	27	0
4	AS	1251	0	1189	31	0
4	AT	1251	0	1189	25	0
4	AW	1251	0	1189	25	0
4	AX	1251	0	1189	27	0
5	AU	977	0	949	39	0
5	AV	977	0	949	39	0
5	AY	977	0	949	41	0
5	AZ	977	0	949	30	0
5	Aa	977	0	949	33	0
5	Ab	977	0	949	28	0
6	R3	1395	0	1428	77	0
6	R4	1395	0	1428	89	0
6	R5	1395	0	1428	89	0
6	S3	1387	0	1417	64	0
6	S4	1387	0	1417	71	0
6	S5	1387	0	1417	68	0
6	T3	1379	0	1406	54	0
6	T4	1379	0	1406	60	0
6	T5	1379	0	1406	60	0
6	U3	1387	0	1417	53	0
6	U4	1387	0	1417	78	0
6	U5	1387	0	1417	53	0
All	All	171990	0	167268	4761	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 4761 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AC:282:THR:H	2:AD:249:ARG:CG	1.60	1.15
2:AB:282:THR:HG23	2:AC:249:ARG:HH21	1.09	1.12
2:AC:281:GLY:CA	2:AD:249:ARG:HG2	1.91	1.00
6:R3:164:MET:HE3	6:R3:168:ASN:HD22	1.27	0.99
2:AG:282:THR:H	2:AH:249:ARG:CG	1.77	0.96

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	219/230 (95%)	199 (91%)	20 (9%)	0	100	100
1	1	219/230 (95%)	196 (90%)	23 (10%)	0	100	100
1	2	219/230 (95%)	195 (89%)	24 (11%)	0	100	100
1	3	219/230 (95%)	201 (92%)	18 (8%)	0	100	100
1	4	219/230 (95%)	196 (90%)	21 (10%)	2 (1%)	14	46
1	5	219/230 (95%)	200 (91%)	19 (9%)	0	100	100
1	6	219/230 (95%)	197 (90%)	22 (10%)	0	100	100
1	7	219/230 (95%)	202 (92%)	17 (8%)	0	100	100
1	8	219/230 (95%)	202 (92%)	17 (8%)	0	100	100
1	9	219/230 (95%)	195 (89%)	23 (10%)	1 (0%)	24	57
1	A	219/230 (95%)	196 (90%)	23 (10%)	0	100	100
1	B	219/230 (95%)	204 (93%)	15 (7%)	0	100	100
1	C	219/230 (95%)	202 (92%)	17 (8%)	0	100	100
1	D	219/230 (95%)	198 (90%)	20 (9%)	1 (0%)	24	57
1	E	219/230 (95%)	200 (91%)	19 (9%)	0	100	100
1	F	219/230 (95%)	196 (90%)	23 (10%)	0	100	100
1	G	219/230 (95%)	201 (92%)	18 (8%)	0	100	100
1	J	219/230 (95%)	194 (89%)	25 (11%)	0	100	100
1	K	219/230 (95%)	193 (88%)	26 (12%)	0	100	100
1	L	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	M	219/230 (95%)	196 (90%)	23 (10%)	0	100	100
1	N	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	O	219/230 (95%)	193 (88%)	25 (11%)	1 (0%)	24	57
1	P	219/230 (95%)	192 (88%)	27 (12%)	0	100	100
1	Q	219/230 (95%)	198 (90%)	21 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	S	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	T	219/230 (95%)	191 (87%)	28 (13%)	0	100	100
1	U	219/230 (95%)	195 (89%)	24 (11%)	0	100	100
1	V	219/230 (95%)	201 (92%)	18 (8%)	0	100	100
1	W	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	X	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	Y	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	Z	219/230 (95%)	197 (90%)	22 (10%)	0	100	100
1	a	219/230 (95%)	196 (90%)	23 (10%)	0	100	100
1	b	219/230 (95%)	200 (91%)	19 (9%)	0	100	100
1	c	219/230 (95%)	196 (90%)	23 (10%)	0	100	100
1	d	219/230 (95%)	199 (91%)	20 (9%)	0	100	100
1	e	219/230 (95%)	199 (91%)	20 (9%)	0	100	100
1	f	219/230 (95%)	197 (90%)	22 (10%)	0	100	100
1	g	219/230 (95%)	200 (91%)	19 (9%)	0	100	100
1	h	219/230 (95%)	201 (92%)	18 (8%)	0	100	100
1	i	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	j	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	k	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	l	219/230 (95%)	199 (91%)	20 (9%)	0	100	100
1	m	219/230 (95%)	197 (90%)	22 (10%)	0	100	100
1	n	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	o	219/230 (95%)	197 (90%)	22 (10%)	0	100	100
1	p	219/230 (95%)	194 (89%)	25 (11%)	0	100	100
1	q	219/230 (95%)	196 (90%)	23 (10%)	0	100	100
1	r	219/230 (95%)	194 (89%)	25 (11%)	0	100	100
1	s	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	t	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	u	219/230 (95%)	195 (89%)	24 (11%)	0	100	100
1	v	219/230 (95%)	196 (90%)	23 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	219/230 (95%)	195 (89%)	24 (11%)	0	100	100
1	x	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	y	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	z	219/230 (95%)	194 (89%)	25 (11%)	0	100	100
2	AA	377/420 (90%)	323 (86%)	54 (14%)	0	100	100
2	AB	377/420 (90%)	324 (86%)	53 (14%)	0	100	100
2	AC	377/420 (90%)	324 (86%)	53 (14%)	0	100	100
2	AD	377/420 (90%)	323 (86%)	54 (14%)	0	100	100
2	AE	377/420 (90%)	322 (85%)	53 (14%)	2 (0%)	24	57
2	AF	377/420 (90%)	324 (86%)	52 (14%)	1 (0%)	36	67
2	AG	377/420 (90%)	323 (86%)	54 (14%)	0	100	100
2	AH	377/420 (90%)	321 (85%)	55 (15%)	1 (0%)	36	67
2	AI	377/420 (90%)	323 (86%)	52 (14%)	2 (0%)	24	57
2	AJ	377/420 (90%)	323 (86%)	54 (14%)	0	100	100
2	AK	377/420 (90%)	323 (86%)	54 (14%)	0	100	100
2	AL	377/420 (90%)	315 (84%)	62 (16%)	0	100	100
3	AM	123/141 (87%)	107 (87%)	16 (13%)	0	100	100
3	AN	123/141 (87%)	107 (87%)	14 (11%)	2 (2%)	7	36
3	AO	123/141 (87%)	108 (88%)	15 (12%)	0	100	100
3	AP	123/141 (87%)	110 (89%)	11 (9%)	2 (2%)	7	36
3	H	123/141 (87%)	109 (89%)	11 (9%)	3 (2%)	4	29
3	I	123/141 (87%)	108 (88%)	13 (11%)	2 (2%)	7	36
4	AQ	153/178 (86%)	136 (89%)	15 (10%)	2 (1%)	9	39
4	AR	153/178 (86%)	137 (90%)	15 (10%)	1 (1%)	18	51
4	AS	153/178 (86%)	132 (86%)	18 (12%)	3 (2%)	6	32
4	AT	153/178 (86%)	137 (90%)	15 (10%)	1 (1%)	18	51
4	AW	153/178 (86%)	134 (88%)	16 (10%)	3 (2%)	6	32
4	AX	153/178 (86%)	135 (88%)	15 (10%)	3 (2%)	6	32
5	AU	126/136 (93%)	112 (89%)	13 (10%)	1 (1%)	16	49
5	AV	126/136 (93%)	114 (90%)	11 (9%)	1 (1%)	16	49
5	AY	126/136 (93%)	113 (90%)	12 (10%)	1 (1%)	16	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AZ	126/136 (93%)	115 (91%)	11 (9%)	0	100	100
5	Aa	126/136 (93%)	115 (91%)	11 (9%)	0	100	100
5	Ab	126/136 (93%)	115 (91%)	11 (9%)	0	100	100
6	R3	177/202 (88%)	142 (80%)	30 (17%)	5 (3%)	4	26
6	R4	177/202 (88%)	142 (80%)	29 (16%)	6 (3%)	3	23
6	R5	177/202 (88%)	141 (80%)	31 (18%)	5 (3%)	4	26
6	S3	176/202 (87%)	142 (81%)	30 (17%)	4 (2%)	5	30
6	S4	176/202 (87%)	143 (81%)	28 (16%)	5 (3%)	4	26
6	S5	176/202 (87%)	142 (81%)	30 (17%)	4 (2%)	5	30
6	T3	175/202 (87%)	143 (82%)	30 (17%)	2 (1%)	11	42
6	T4	175/202 (87%)	146 (83%)	27 (15%)	2 (1%)	11	42
6	T5	175/202 (87%)	143 (82%)	30 (17%)	2 (1%)	11	42
6	U3	176/202 (87%)	143 (81%)	27 (15%)	6 (3%)	3	23
6	U4	176/202 (87%)	139 (79%)	32 (18%)	5 (3%)	4	26
6	U5	176/202 (87%)	142 (81%)	29 (16%)	5 (3%)	4	26
All	All	22188/23994 (92%)	19565 (88%)	2536 (11%)	87 (0%)	31	62

5 of 87 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AP	50	ASP
6	R3	168	ASN
6	S3	73	PRO
6	U3	141	PRO
6	U3	174	ALA

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	186/191 (97%)	184 (99%)	2 (1%)	65	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	186/191 (97%)	184 (99%)	2 (1%)	65	75
1	2	186/191 (97%)	185 (100%)	1 (0%)	81	81
1	3	186/191 (97%)	186 (100%)	0	100	100
1	4	186/191 (97%)	185 (100%)	1 (0%)	81	81
1	5	186/191 (97%)	184 (99%)	2 (1%)	65	75
1	6	186/191 (97%)	186 (100%)	0	100	100
1	7	186/191 (97%)	183 (98%)	3 (2%)	55	71
1	8	186/191 (97%)	186 (100%)	0	100	100
1	9	186/191 (97%)	184 (99%)	2 (1%)	65	75
1	A	186/191 (97%)	186 (100%)	0	100	100
1	B	186/191 (97%)	184 (99%)	2 (1%)	65	75
1	C	186/191 (97%)	186 (100%)	0	100	100
1	D	186/191 (97%)	185 (100%)	1 (0%)	81	81
1	E	186/191 (97%)	184 (99%)	2 (1%)	65	75
1	F	186/191 (97%)	186 (100%)	0	100	100
1	G	186/191 (97%)	183 (98%)	3 (2%)	55	71
1	J	186/191 (97%)	186 (100%)	0	100	100
1	K	186/191 (97%)	186 (100%)	0	100	100
1	L	186/191 (97%)	185 (100%)	1 (0%)	81	81
1	M	186/191 (97%)	186 (100%)	0	100	100
1	N	186/191 (97%)	186 (100%)	0	100	100
1	O	186/191 (97%)	184 (99%)	2 (1%)	65	75
1	P	186/191 (97%)	186 (100%)	0	100	100
1	Q	186/191 (97%)	184 (99%)	2 (1%)	65	75
1	R	186/191 (97%)	186 (100%)	0	100	100
1	S	186/191 (97%)	186 (100%)	0	100	100
1	T	186/191 (97%)	185 (100%)	1 (0%)	81	81
1	U	186/191 (97%)	186 (100%)	0	100	100
1	V	186/191 (97%)	185 (100%)	1 (0%)	81	81
1	W	186/191 (97%)	186 (100%)	0	100	100
1	X	186/191 (97%)	186 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	186/191 (97%)	186 (100%)	0	100	100
1	Z	186/191 (97%)	185 (100%)	1 (0%)	81	81
1	a	186/191 (97%)	186 (100%)	0	100	100
1	b	186/191 (97%)	186 (100%)	0	100	100
1	c	186/191 (97%)	186 (100%)	0	100	100
1	d	186/191 (97%)	186 (100%)	0	100	100
1	e	186/191 (97%)	185 (100%)	1 (0%)	81	81
1	f	186/191 (97%)	186 (100%)	0	100	100
1	g	186/191 (97%)	186 (100%)	0	100	100
1	h	186/191 (97%)	185 (100%)	1 (0%)	81	81
1	i	186/191 (97%)	186 (100%)	0	100	100
1	j	186/191 (97%)	184 (99%)	2 (1%)	65	75
1	k	186/191 (97%)	186 (100%)	0	100	100
1	l	186/191 (97%)	186 (100%)	0	100	100
1	m	186/191 (97%)	186 (100%)	0	100	100
1	n	186/191 (97%)	185 (100%)	1 (0%)	81	81
1	o	186/191 (97%)	186 (100%)	0	100	100
1	p	186/191 (97%)	185 (100%)	1 (0%)	81	81
1	q	186/191 (97%)	184 (99%)	2 (1%)	65	75
1	r	186/191 (97%)	185 (100%)	1 (0%)	81	81
1	s	186/191 (97%)	185 (100%)	1 (0%)	81	81
1	t	186/191 (97%)	186 (100%)	0	100	100
1	u	186/191 (97%)	184 (99%)	2 (1%)	65	75
1	v	186/191 (97%)	185 (100%)	1 (0%)	81	81
1	w	186/191 (97%)	185 (100%)	1 (0%)	81	81
1	x	186/191 (97%)	185 (100%)	1 (0%)	81	81
1	y	186/191 (97%)	186 (100%)	0	100	100
1	z	186/191 (97%)	185 (100%)	1 (0%)	81	81
2	AA	311/339 (92%)	310 (100%)	1 (0%)	86	83
2	AB	311/339 (92%)	311 (100%)	0	100	100
2	AC	311/339 (92%)	310 (100%)	1 (0%)	86	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AD	311/339 (92%)	304 (98%)	7 (2%)	44	65
2	AE	311/339 (92%)	311 (100%)	0	100	100
2	AF	311/339 (92%)	307 (99%)	4 (1%)	61	73
2	AG	311/339 (92%)	310 (100%)	1 (0%)	86	83
2	AH	311/339 (92%)	305 (98%)	6 (2%)	50	68
2	AI	311/339 (92%)	309 (99%)	2 (1%)	78	80
2	AJ	311/339 (92%)	309 (99%)	2 (1%)	78	80
2	AK	311/339 (92%)	310 (100%)	1 (0%)	86	83
2	AL	311/339 (92%)	306 (98%)	5 (2%)	55	71
3	AM	114/128 (89%)	114 (100%)	0	100	100
3	AN	114/128 (89%)	111 (97%)	3 (3%)	40	64
3	AO	114/128 (89%)	114 (100%)	0	100	100
3	AP	114/128 (89%)	112 (98%)	2 (2%)	51	70
3	H	114/128 (89%)	112 (98%)	2 (2%)	51	70
3	I	114/128 (89%)	112 (98%)	2 (2%)	51	70
4	AQ	134/153 (88%)	131 (98%)	3 (2%)	45	66
4	AR	134/153 (88%)	129 (96%)	5 (4%)	30	57
4	AS	134/153 (88%)	131 (98%)	3 (2%)	45	66
4	AT	134/153 (88%)	132 (98%)	2 (2%)	57	72
4	AW	134/153 (88%)	131 (98%)	3 (2%)	45	66
4	AX	134/153 (88%)	132 (98%)	2 (2%)	57	72
5	AU	113/116 (97%)	111 (98%)	2 (2%)	51	70
5	AV	113/116 (97%)	111 (98%)	2 (2%)	51	70
5	AY	113/116 (97%)	112 (99%)	1 (1%)	70	76
5	AZ	113/116 (97%)	111 (98%)	2 (2%)	51	70
5	Aa	113/116 (97%)	111 (98%)	2 (2%)	51	70
5	Ab	113/116 (97%)	110 (97%)	3 (3%)	39	63
6	R3	149/168 (89%)	142 (95%)	7 (5%)	23	51
6	R4	149/168 (89%)	140 (94%)	9 (6%)	17	45
6	R5	149/168 (89%)	147 (99%)	2 (1%)	61	73
6	S3	148/168 (88%)	145 (98%)	3 (2%)	48	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	S4	148/168 (88%)	145 (98%)	3 (2%)	48	67
6	S5	148/168 (88%)	146 (99%)	2 (1%)	59	72
6	T3	147/168 (88%)	144 (98%)	3 (2%)	48	67
6	T4	147/168 (88%)	141 (96%)	6 (4%)	27	54
6	T5	147/168 (88%)	142 (97%)	5 (3%)	32	59
6	U3	148/168 (88%)	140 (95%)	8 (5%)	20	47
6	U4	148/168 (88%)	133 (90%)	15 (10%)	7	29
6	U5	148/168 (88%)	143 (97%)	5 (3%)	32	59
All	All	18834/19926 (94%)	18652 (99%)	182 (1%)	65	76

5 of 182 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	AS	95	LYS
6	U4	19	ASP
4	AT	95	LYS
6	R4	186	VAL
6	U4	157	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 219 such sidechains are listed below:

Mol	Chain	Res	Type
2	AG	202	ASN
2	AK	102	GLN
6	U4	155	ASN
2	AH	44	ASN
2	AI	191	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

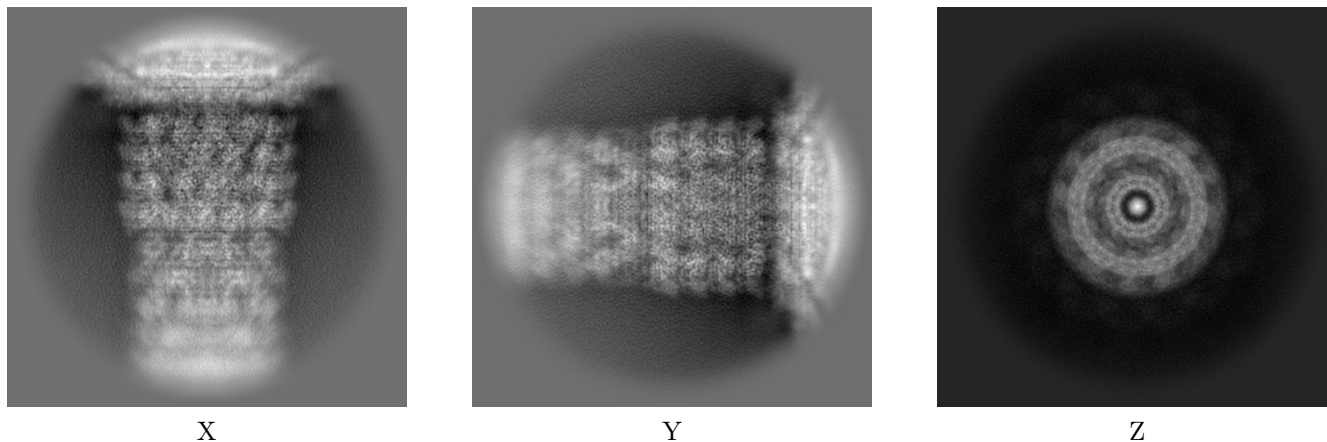
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29503. These allow visual inspection of the internal detail of the map and identification of artifacts.

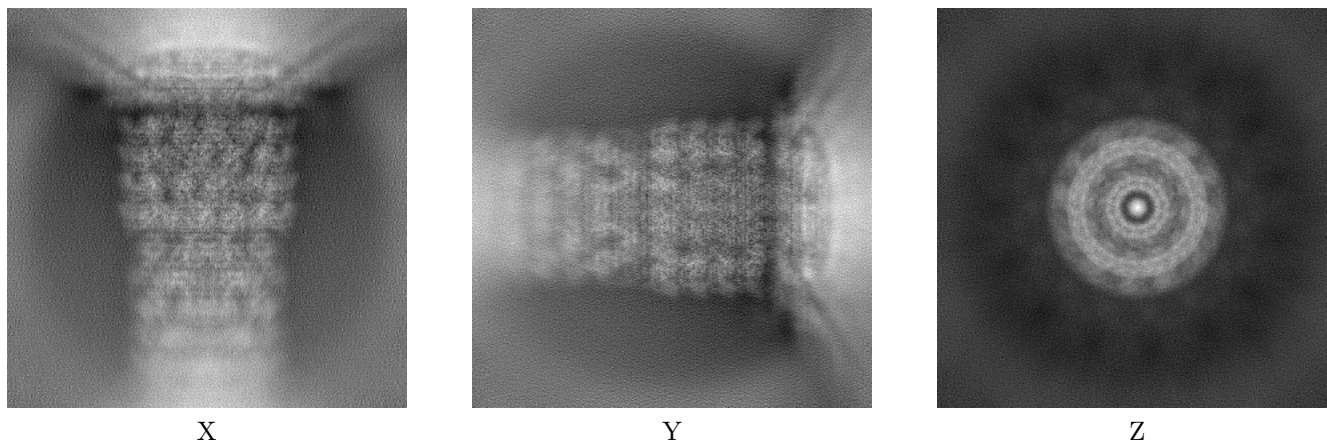
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



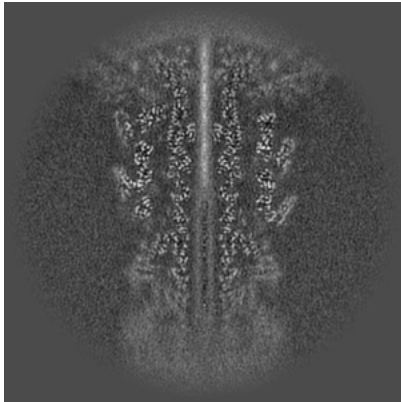
#### 6.1.2 Raw map



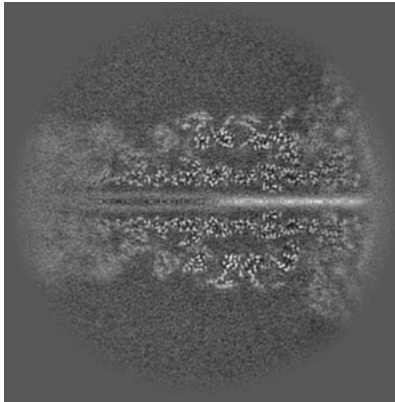
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

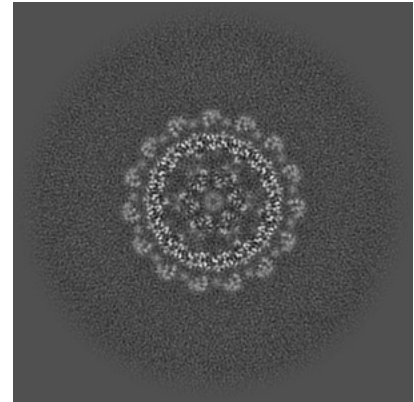
### 6.2.1 Primary map



X Index: 224

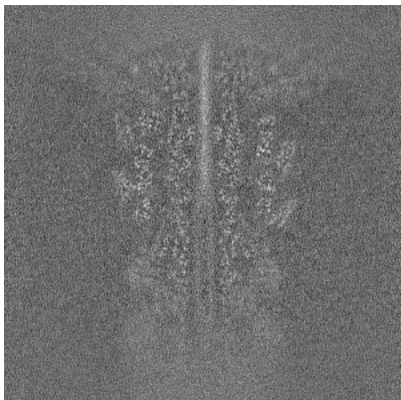


Y Index: 224

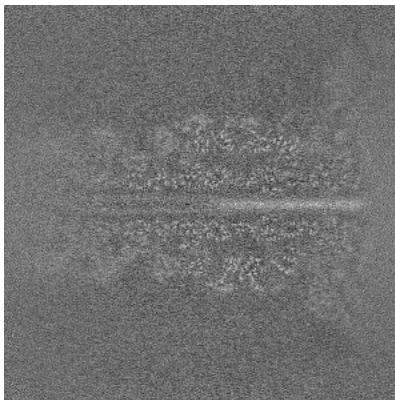


Z Index: 224

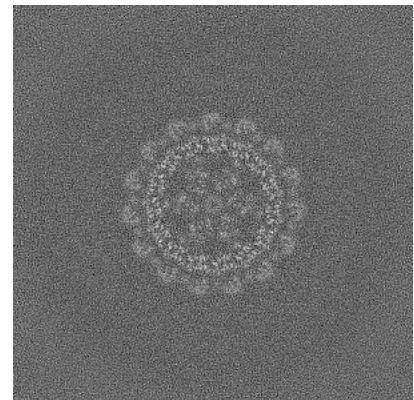
### 6.2.2 Raw map



X Index: 224



Y Index: 224

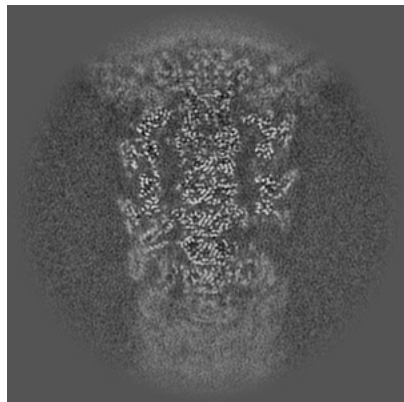


Z Index: 224

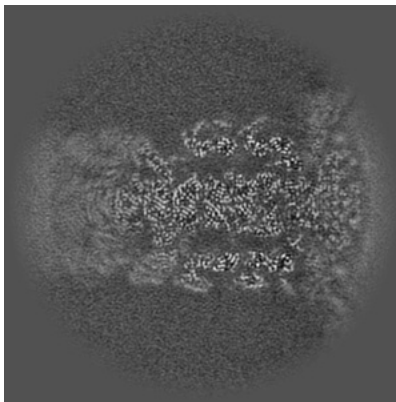
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

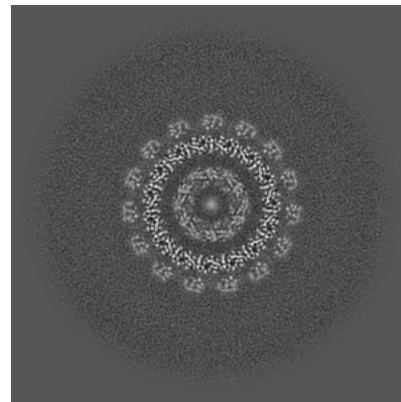
### 6.3.1 Primary map



X Index: 246

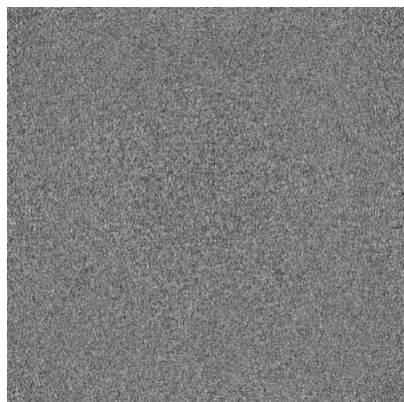


Y Index: 246

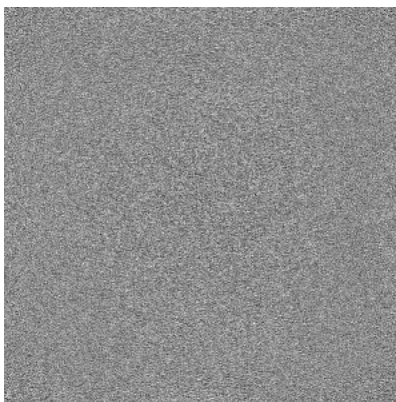


Z Index: 284

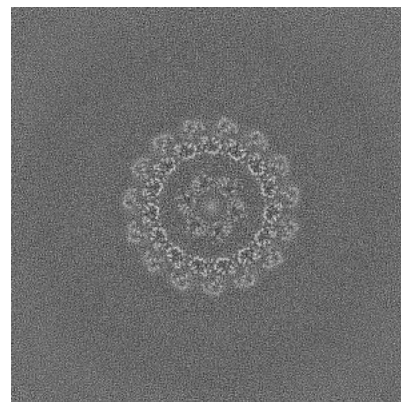
### 6.3.2 Raw map



X Index: 0



Y Index: 0

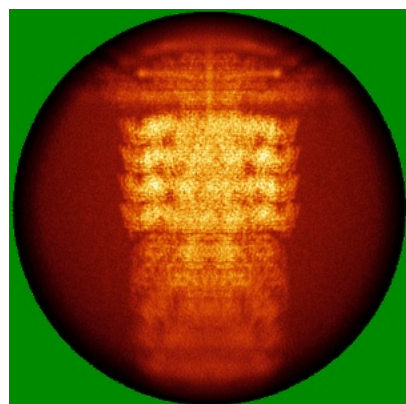


Z Index: 249

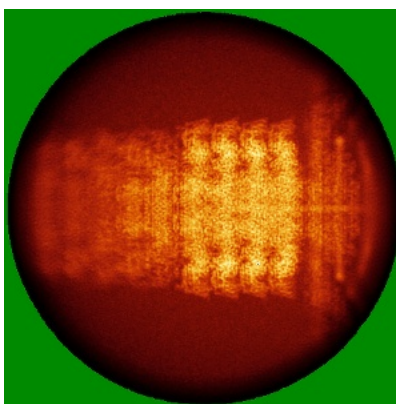
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

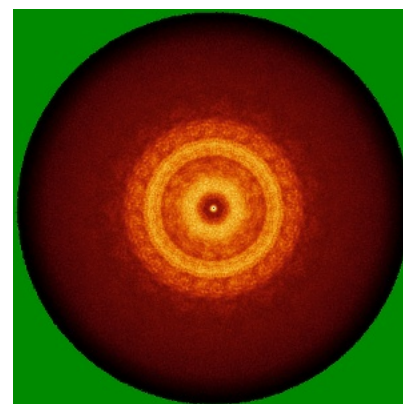
### 6.4.1 Primary map



X

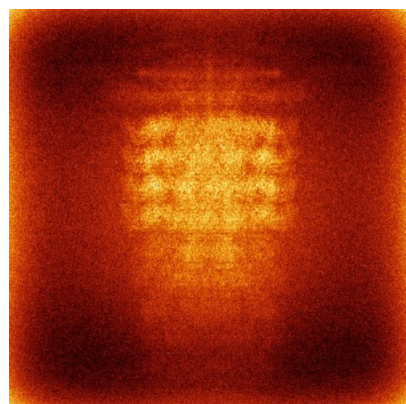


Y

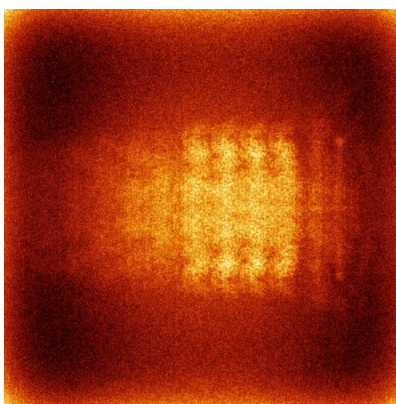


Z

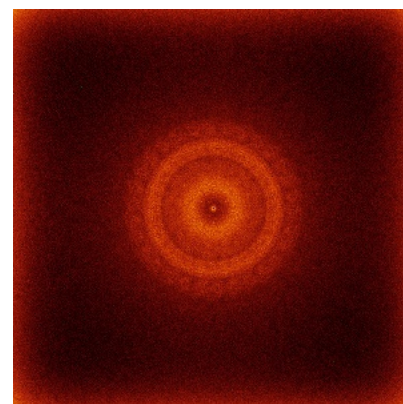
### 6.4.2 Raw map



X



Y

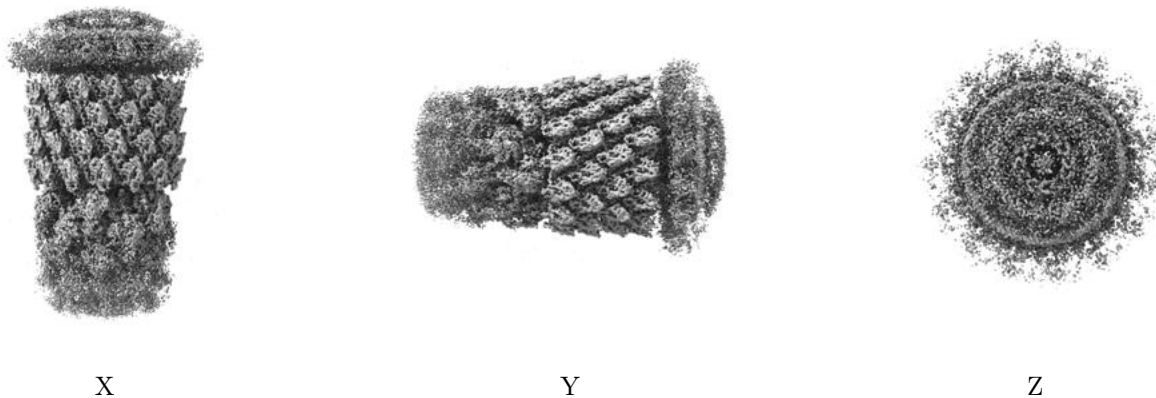


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

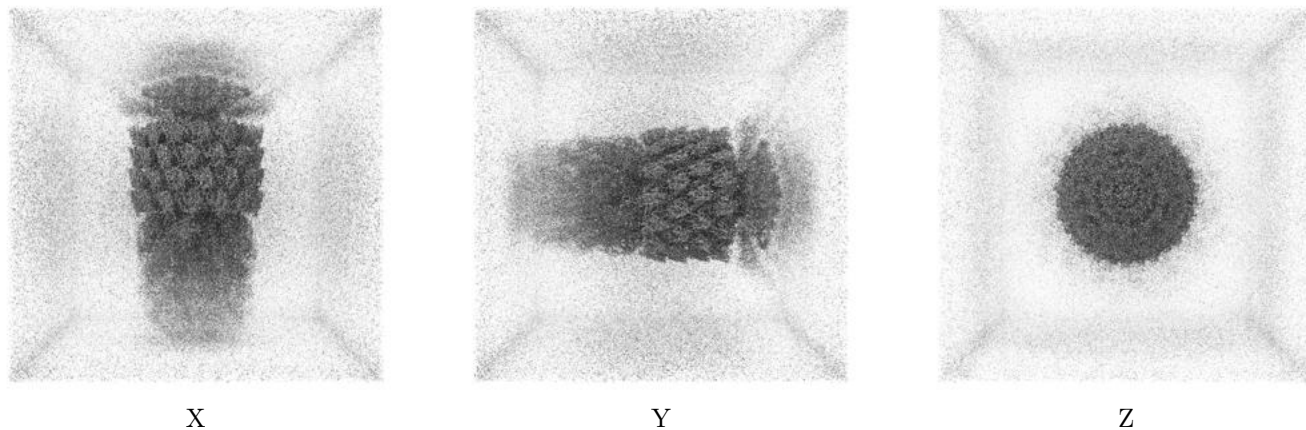
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

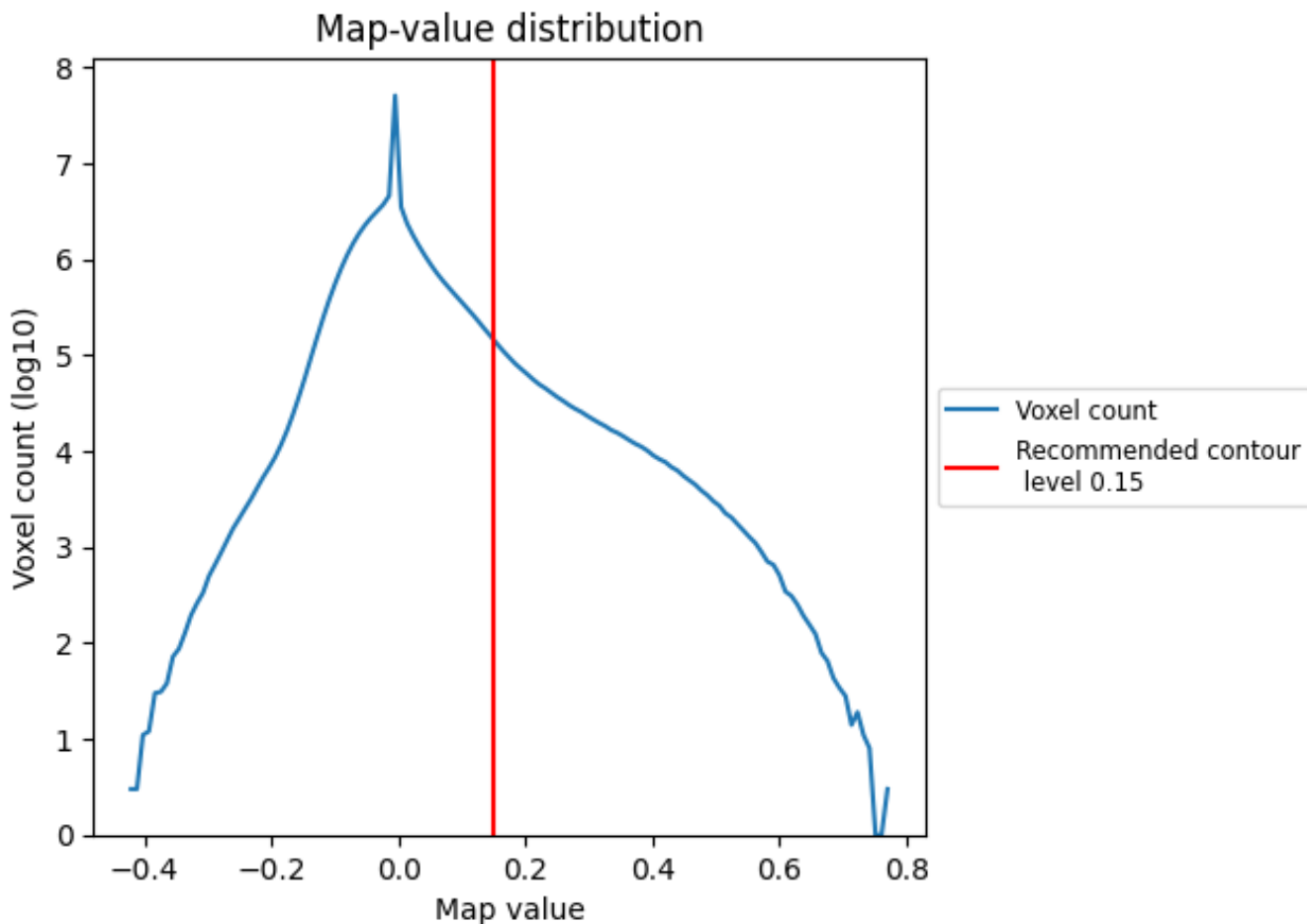
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

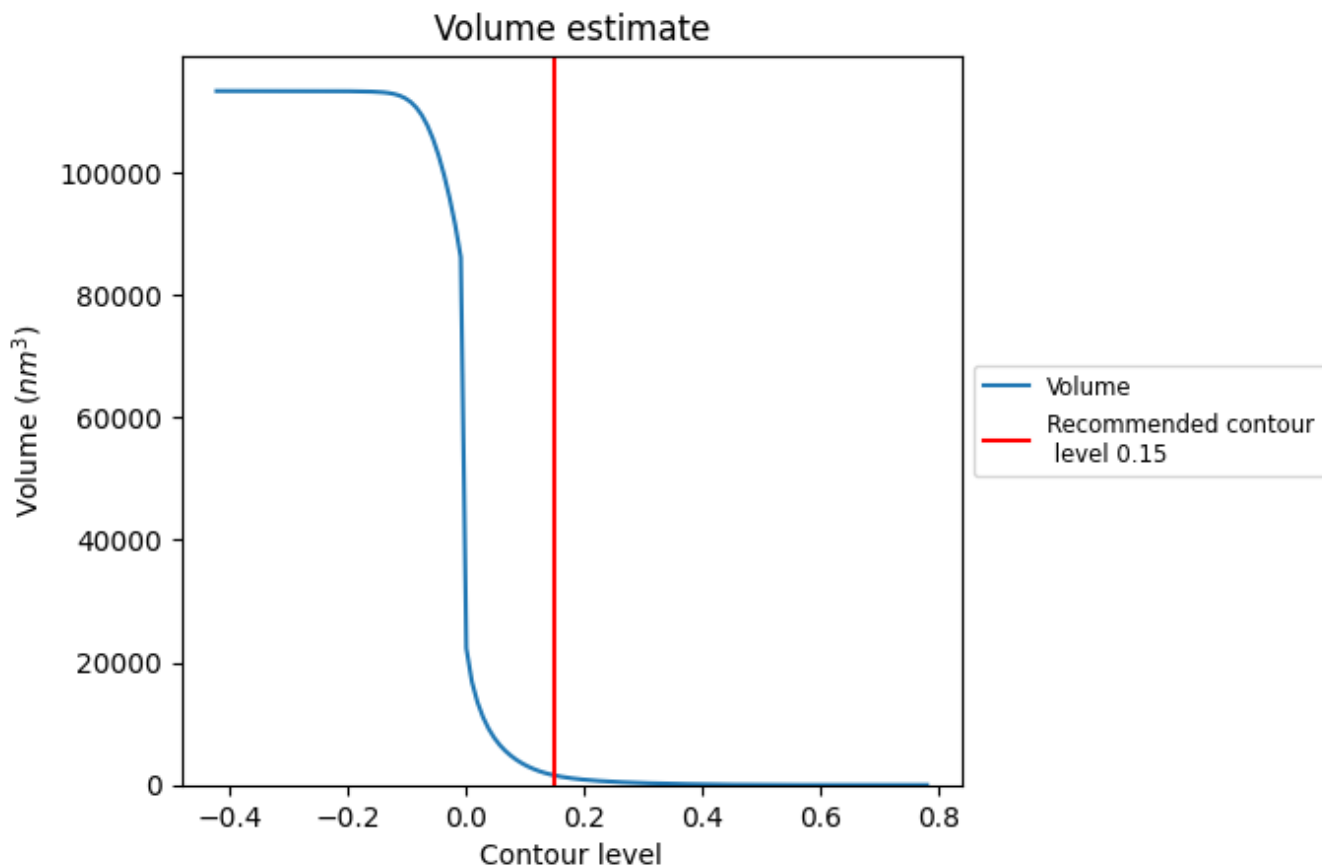
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

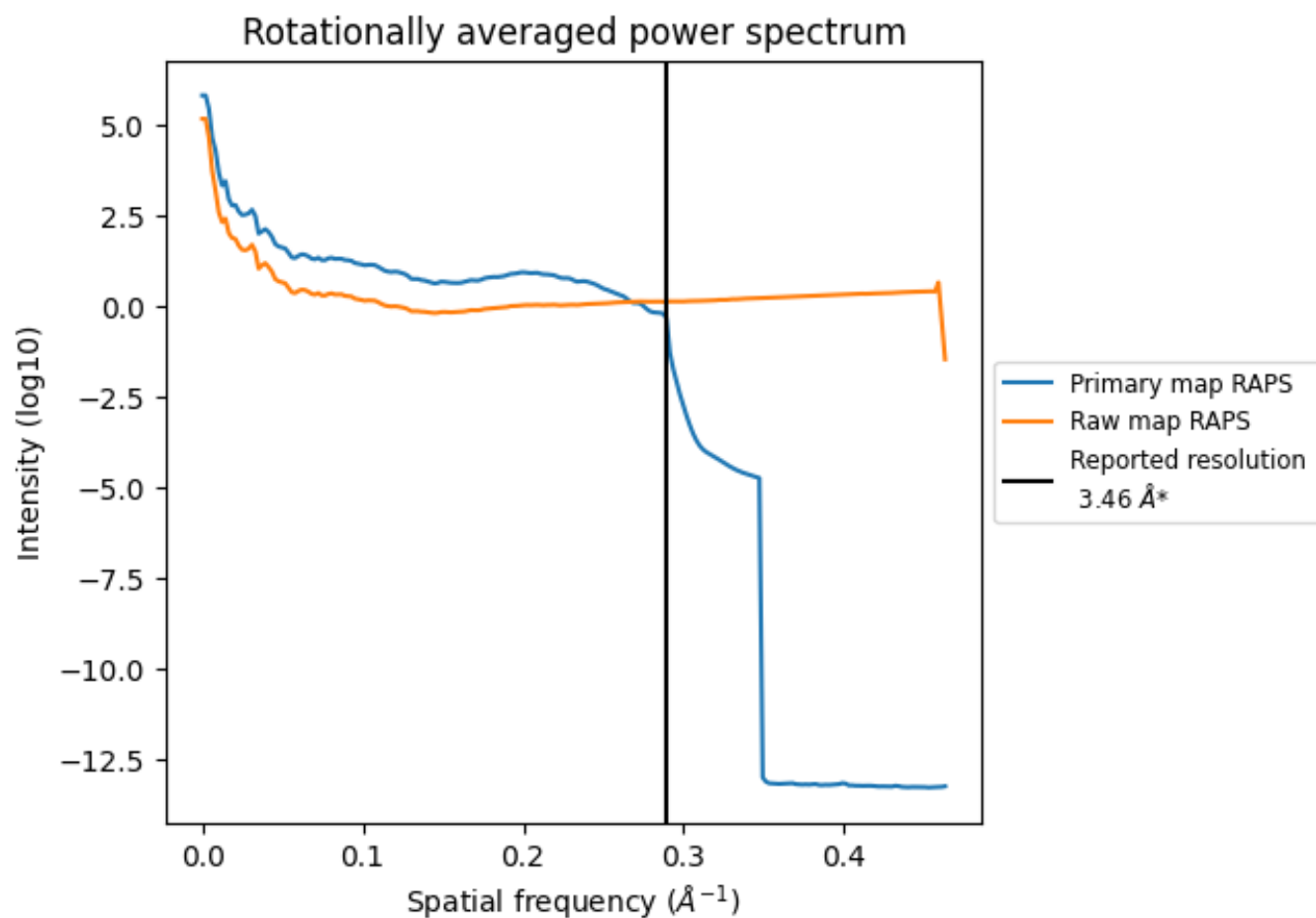
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1570  $\text{nm}^3$ ; this corresponds to an approximate mass of 1418 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

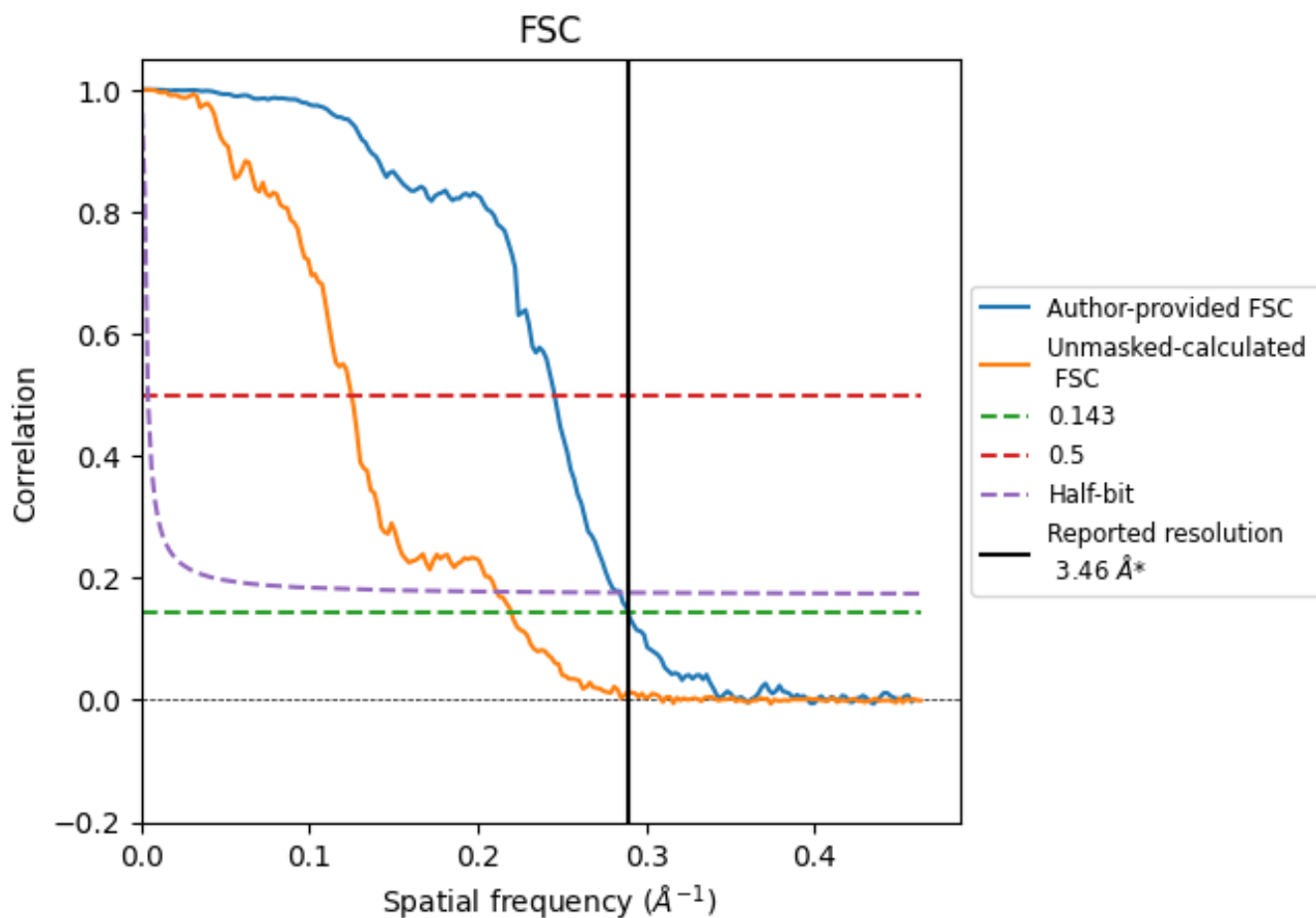


\*Reported resolution corresponds to spatial frequency of 0.289 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.289 Å<sup>-1</sup>

## 8.2 Resolution estimates

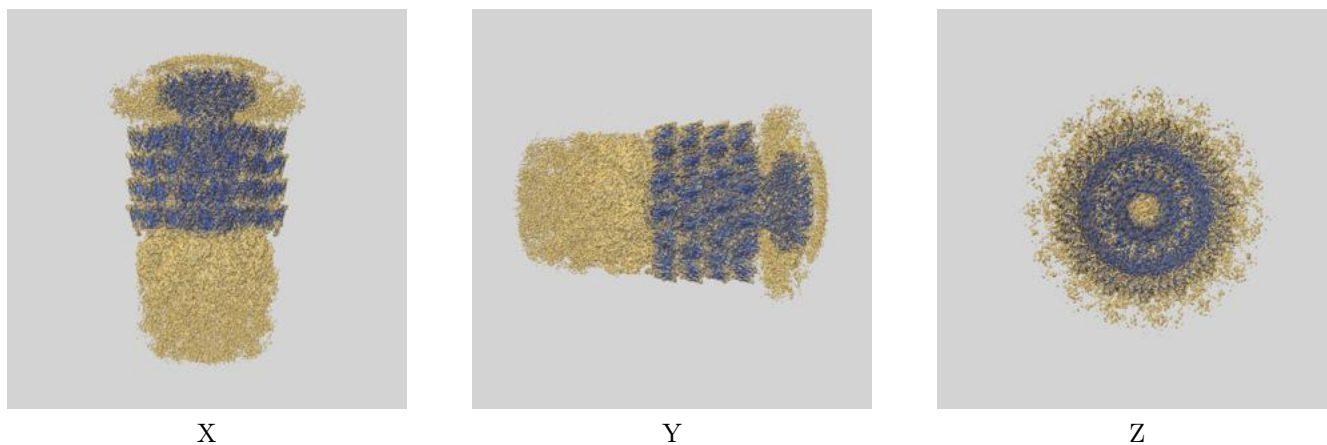
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	3.46	4.07	3.51
Unmasked-calculated*	4.55	8.01	4.74

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.55 differs from the reported value 3.46 by more than 10 %

## 9 Map-model fit [i](#)

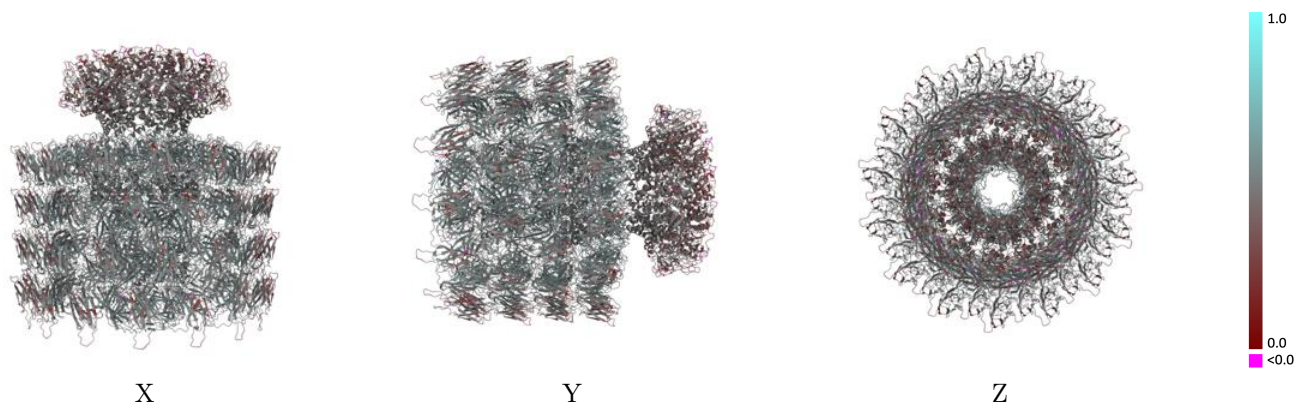
This section contains information regarding the fit between EMDB map EMD-29503 and PDB model 8FWE. Per-residue inclusion information can be found in section [3](#) on page [13](#).

### 9.1 Map-model overlay [i](#)



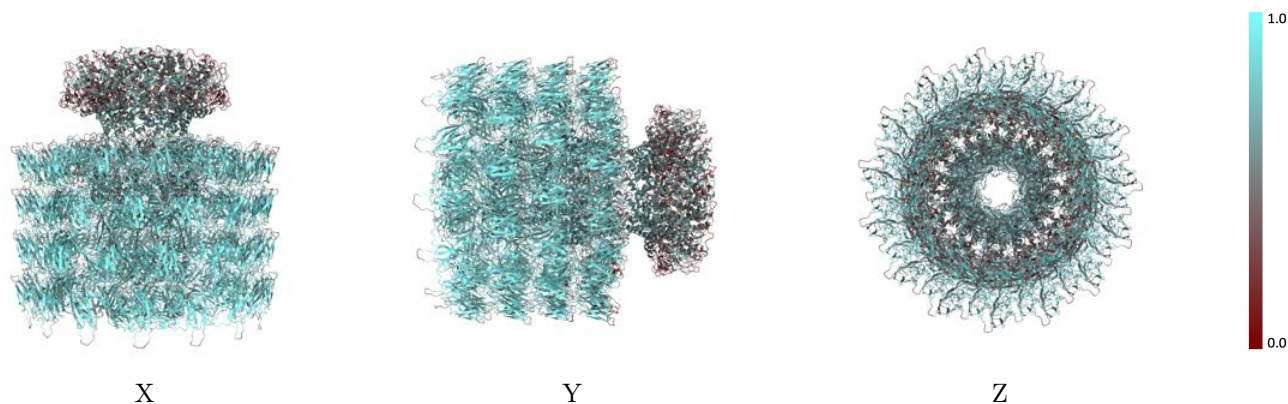
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



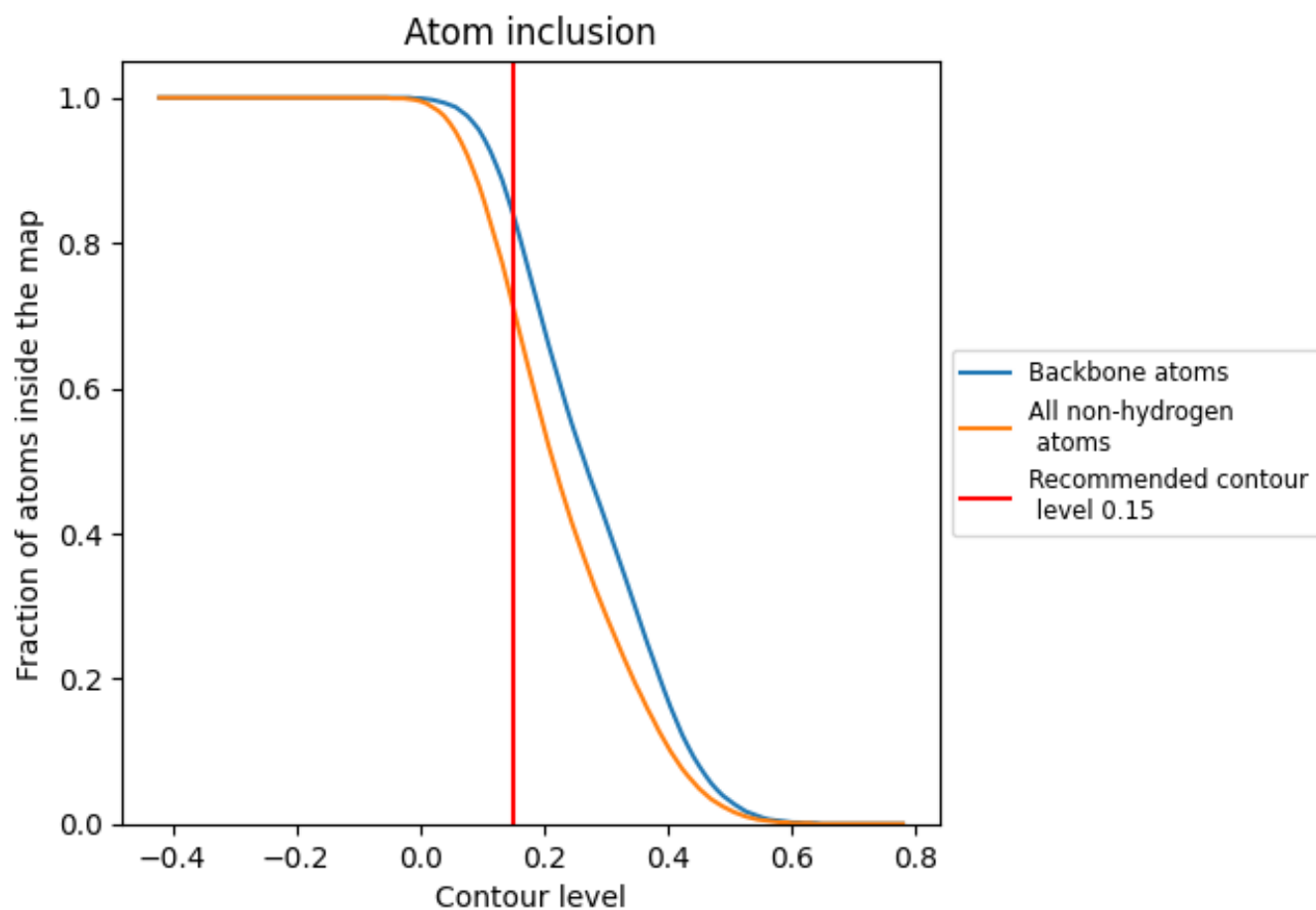
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7140	 0.4750
0	 0.7990	 0.4700
1	 0.8180	 0.4950
2	 0.8130	 0.4880
3	 0.7890	 0.4700
4	 0.7910	 0.4670
5	 0.7960	 0.4710
6	 0.7940	 0.4650
7	 0.7830	 0.4660
8	 0.7880	 0.4720
9	 0.7860	 0.4660
A	 0.8000	 0.4650
AA	 0.5160	 0.4230
AB	 0.4750	 0.3970
AC	 0.4810	 0.4030
AD	 0.5070	 0.4190
AE	 0.5210	 0.4250
AF	 0.4770	 0.4000
AG	 0.4870	 0.4030
AH	 0.5080	 0.4200
AI	 0.5170	 0.4240
AJ	 0.4730	 0.3980
AK	 0.4860	 0.4020
AL	 0.5120	 0.4200
AM	 0.7670	 0.5320
AN	 0.7700	 0.5300
AO	 0.7740	 0.5260
AP	 0.7530	 0.5310
AQ	 0.7740	 0.5200
AR	 0.7680	 0.5160
AS	 0.7750	 0.5200
AT	 0.7660	 0.5180
AU	 0.7650	 0.5150
AV	 0.7680	 0.5180
AW	 0.7660	 0.5220























































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Chain	Atom inclusion	Q-score
AX	 0.7620	 0.5180
AY	 0.7630	 0.5180
AZ	 0.7570	 0.5220
Aa	 0.7570	 0.5220
Ab	 0.7580	 0.5210
B	 0.7850	 0.4660
C	 0.7910	 0.4700
D	 0.7800	 0.4620
E	 0.7980	 0.4720
F	 0.7940	 0.4650
G	 0.7800	 0.4670
H	 0.7550	 0.5280
I	 0.7530	 0.5280
J	 0.7510	 0.4910
K	 0.7490	 0.4920
L	 0.7520	 0.4840
M	 0.7250	 0.4830
N	 0.7210	 0.4810
O	 0.7580	 0.4920
P	 0.7450	 0.4900
Q	 0.7510	 0.4830
R	 0.7240	 0.4830
R3	 0.7010	 0.5040
R4	 0.6930	 0.5070
R5	 0.6940	 0.5030
S	 0.7250	 0.4810
S3	 0.6950	 0.5080
S4	 0.6940	 0.5100
S5	 0.6880	 0.5100
T	 0.7570	 0.4890
T3	 0.6420	 0.5120
T4	 0.6410	 0.5090
T5	 0.6440	 0.5110
U	 0.7530	 0.4920
U3	 0.6420	 0.4980
U4	 0.6400	 0.5010
U5	 0.6430	 0.5000
V	 0.7550	 0.4880
W	 0.7260	 0.4840
X	 0.7240	 0.4820
Y	 0.8100	 0.4960
Z	 0.7940	 0.4910

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Chain	Atom inclusion	Q-score
a	 0.8080	 0.4890
b	 0.7970	 0.4830
c	 0.7940	 0.4890
d	 0.8080	 0.4920
e	 0.7930	 0.4910
f	 0.8060	 0.4890
g	 0.7990	 0.4830
h	 0.7930	 0.4900
i	 0.8090	 0.4930
j	 0.7910	 0.4900
k	 0.8110	 0.4910
l	 0.7950	 0.4850
m	 0.7920	 0.4910
n	 0.8290	 0.4920
o	 0.8260	 0.4980
p	 0.8170	 0.4910
q	 0.8240	 0.4930
r	 0.8110	 0.4880
s	 0.8260	 0.4900
t	 0.8280	 0.4980
u	 0.8180	 0.4930
v	 0.8190	 0.4930
w	 0.8180	 0.4880
x	 0.8250	 0.4910
y	 0.8210	 0.4980
z	 0.8210	 0.4930